

75th MORSS 712CD Cover Page

12-14 June 2007, at US Naval Academy, Annapolis, MD

If you would like your presentation included in the 75th MORSS Final Report CD it must:

1. Be unclassified, approved for public release, distribution unlimited, and is exempt from US export licensing and other export approvals including the International Traffic in Arms Regulations (22CFR120 et.seq.),
2. include MORSS Form 712CD as the first page of the presentation and
3. a MORSS form 712 A or B must be in the MORSS Office no later than **14 June 2007**.

Author Request (To be completed by applicant) - The following author(s) request authority to disclose the following presentation in the MORSS Final Report, for inclusion on the MORSS CD and/or posting on the MORSS web site.

Name of Principal Author and all other author(s): Thomas A. Donnelly

Principal Author's Organization and address: U.S. Army Edgewood CB Center, AMSRD-ECB-RT-IM, 5183 Blackhawk Rd., E5951/214-C,

Aberdeen Proving Ground, MD 21010-5424 Phone: 410-436-2571 Email: thomas.a.donnelly@us.army.mil

Original title on 712 A/B: Leveraging Process Knowledge to Improve Modeling of Evaporation Rate Data for Agent Fate Wind Tunnels

(Please use the same title listed on MORSS Form 712 A/B. If the title was changed please list the revised title below.) Revised title:

Presented in: WG(s) #2 & #25, CG _____, Special Session _____,

Demonstration, _____, Tutorial, _____ or Focus Session # _____

The following presentation is believed to be: unclassified, approved for public release, distribution unlimited, and is exempt from US export licensing and other export approvals including the International Traffic in Arms Regulations (22CFR120 et.seq.)

Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE 13 JUN 2007		2. REPORT TYPE N/A		3. DATES COVERED -	
4. TITLE AND SUBTITLE Leveraging Process Knowledge to Improve Modeling of Evaporation Rate Data for Agent Fate Wind Tunnels				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Edgewood Chemical Biological Center 5183 Blackhawk Road, ATTN: AMSRD-ECB-RT-IM Aberdeen proving Ground, MD 21010-5424				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release, distribution unlimited					
13. SUPPLEMENTARY NOTES See also ADM202526. Military Operations Research Society Symposium (75th) Held in Annapolis, Maryland on June 12-14, 2007., The original document contains color images.					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 45	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

UNCLASSIFIED/UNLIMITED

Leveraging Process Knowledge to Improve Modeling of Evaporation Rate Data for Agent Fate Wind Tunnels

*Presented at
75th MORS Symposium
13 June 2007*

Thomas A. Donnelly, Ph.D.
R&T Directorate, ECBC

DISCLAIMER: The findings presented in this briefing are not to be construed as an official Department of the Army position unless so designated by other authorizing documents.



Edgewood Chemical Biological Center
5183 Blackhawk Road, ATTN: AMSRD-ECB-RT-IM
Aberdeen Proving Ground, Maryland, USA 21010-5424

Email: thomas.a.donnelly@us.army.mil
Phone: (410) 436-2571
FAX: (410) 436-2165

UNCLASSIFIED/UNLIMITED



ECBC

Purpose of Talk

- Demonstrate how the modeling (regression analysis) of evaporation rate data can be improved by rescaling the variables based on knowledge of the process
- Describe how running the experimental design trials in specific randomized blocks – as compared to running the planned trials in a haphazard order – facilitates:
 - A sequential model building process
 - Identifying when running more trials adds little new information



Summary

- Rescaling the variables using knowledge of the physics reduces the complexity of the model required to adequately fit the data
 - Before rescaling, a 10-term quadratic model was needed
 - After rescaling, a 4-term linear model is all that is needed
- Extrapolated predictions for checkpoints within the 5-cm tunnel data validate “nearby” extrapolation with the physics-based linear model
- For the physics-based linear model “farther out” extrapolations are more plausible than those of the empirical model.
 - Note that these “farther out” conditions are beyond the practical range of the wind tunnels and that these predictions have not been validated.



Summary

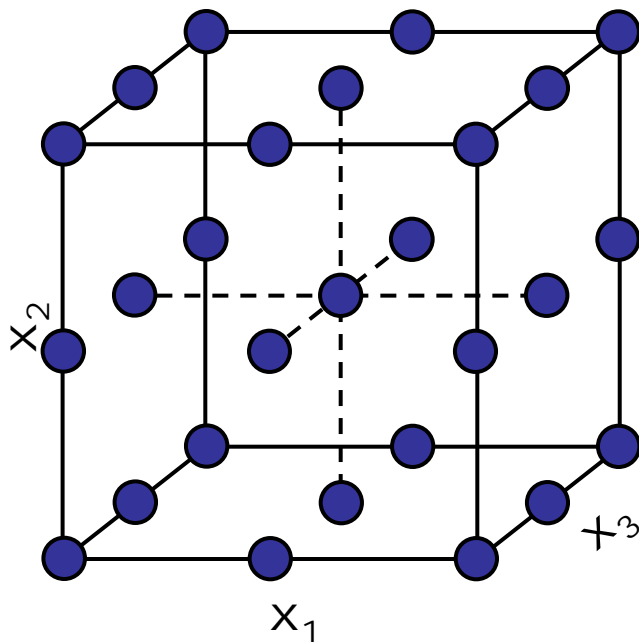
- Although the same level of reduction of the number of required trials seen for HD on glass may not hold true for other agents and/or substrates, results point to importance of running trials in a sequence of blocks that support increasingly complex models.
- Combining the data for the 5-cm and 10-cm tunnels shows that the “tunnel effect” - although statistically significant - is dwarfed by the effects of the Temperature, Wind Velocity and Drop Size which are 5X to 14X as large. For HD on glass, the behavior of the two tunnels appears quite similar.



Data for HD on Glass Came from Two Sources

- 5-cm ECBC tunnel data
 - 19 unique trials – with one observation for each – i.e. no replicates
- 10-cm Czech tunnel data
 - 13 unique trials with 34 observations – eight 2X, four 3X and one 6X
- In both cases the original plan called for the running of a “validation design” - 27 unique trials making up the 3 X 3 X 3 full-factorial design

3 X 3 X 3 Full-Factorial Design and Empirical Model Terms It Can Support

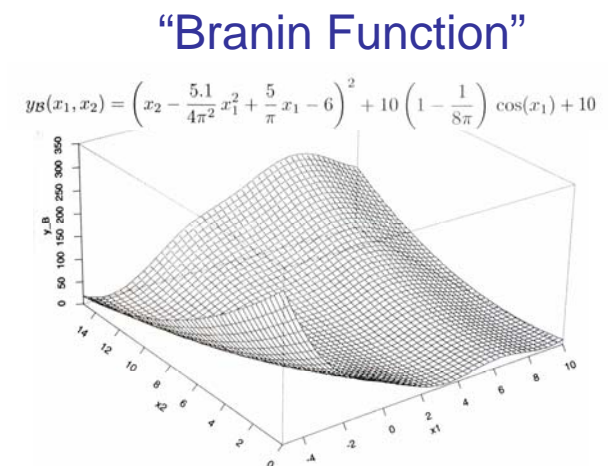
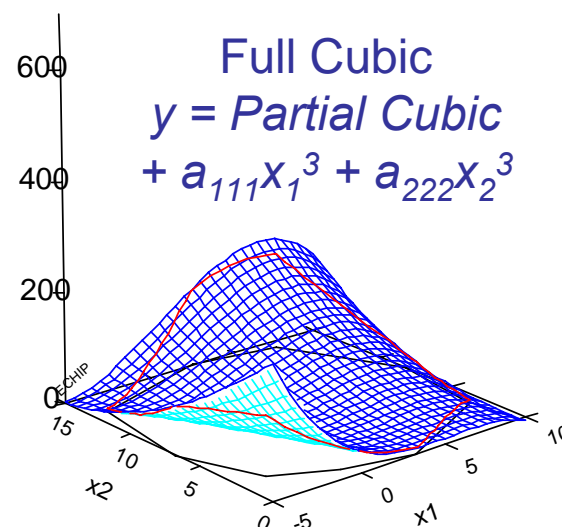
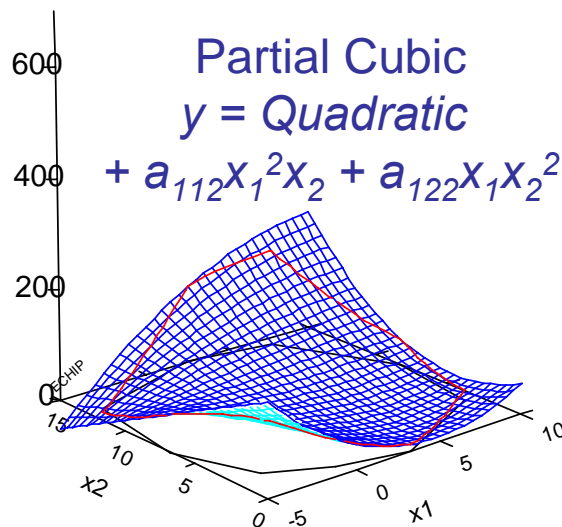
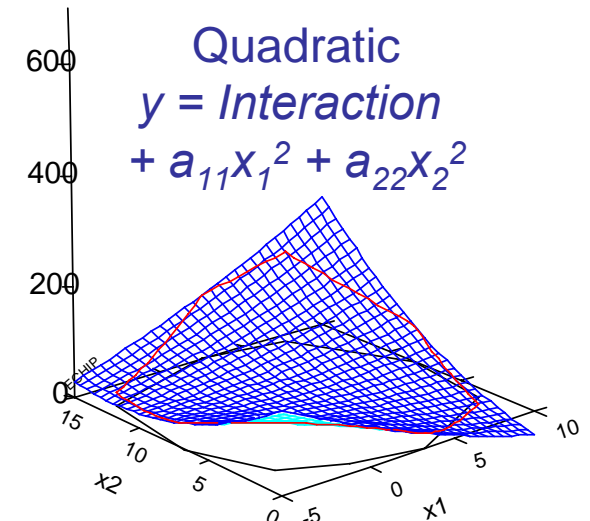
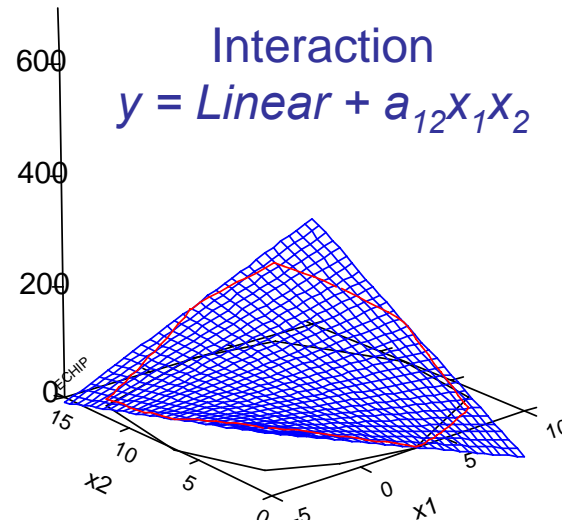
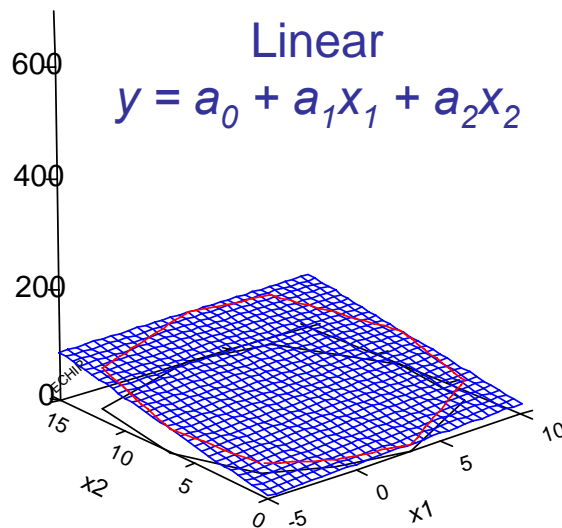


$$\begin{aligned}
 y = & a_0 + a_1x_1 + a_2x_2 + a_3x_3 \\
 & + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 \\
 & + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2 \\
 & + a_{123}x_1x_2x_3 \\
 & + a_{112}x_1^2x_2 + a_{122}x_1x_2^2 + a_{113}x_1^2x_3 \\
 & + a_{133}x_1x_3^2 + a_{223}x_2^2x_3 + a_{233}x_2x_3^2
 \end{aligned}$$

constant + linear
 + 2-way interactions
 + curvature terms
 + 3-way interaction
 + partial cubic terms

Because this design does not have 4 levels/variable, it cannot be used to fit full cubic terms such as $a_{111}x_1^3$, $a_{222}x_2^3$ and $a_{333}x_3^3$.

Comparing Surfaces for Increasingly Complex Polynomials Fit to Data from the Branin Function

FIGURE C.1. The Branin function on $[-5, 10] \times [0, 15]$

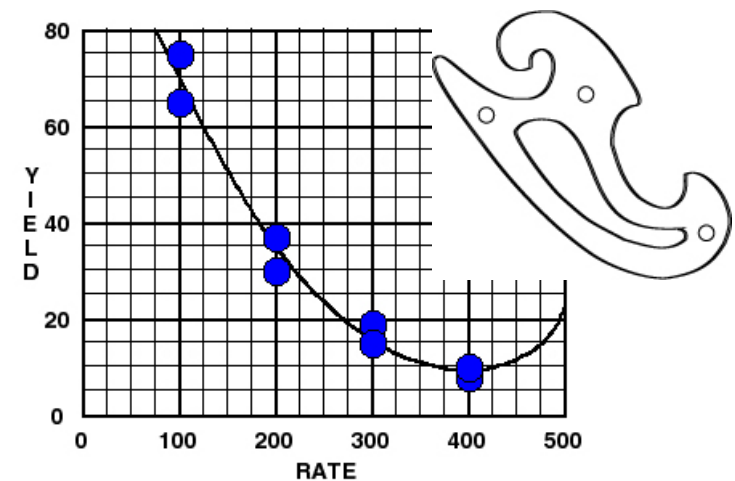
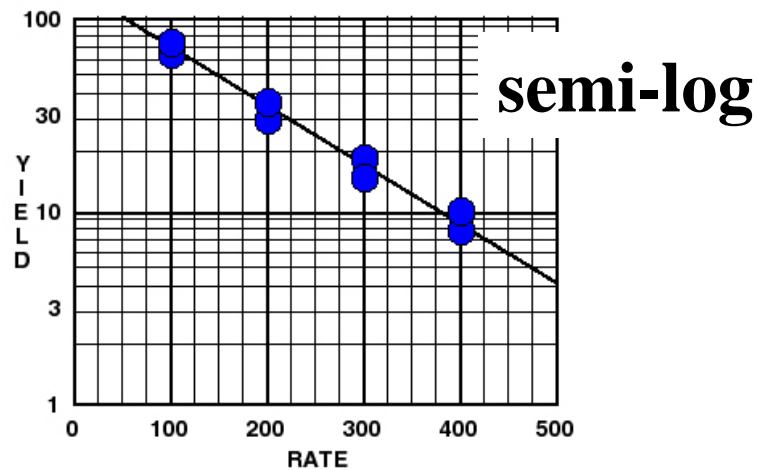
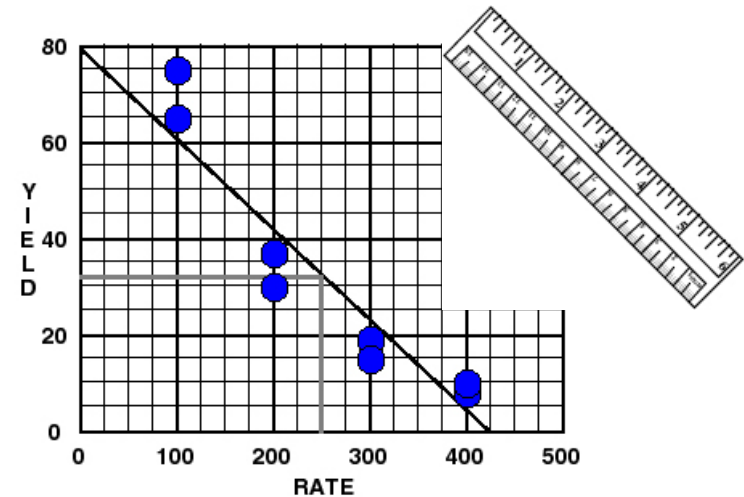
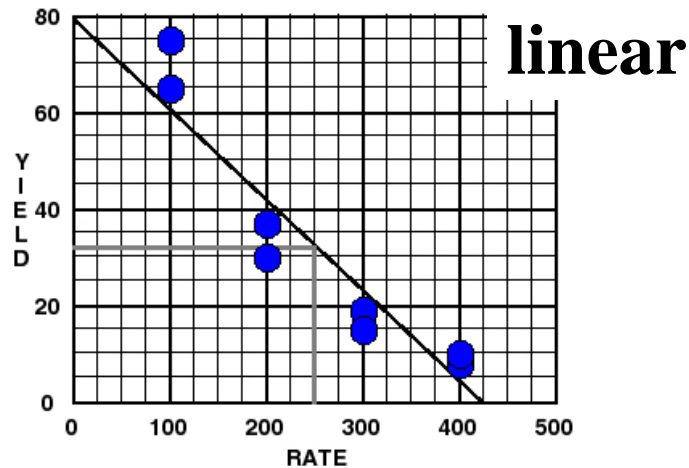
Of these models, the *full cubic* best approximates the Branin function, but still cannot represent the ripples visible on edges of the last plot.

Data Transformations – Why Do Them?

- Remedy for lack of fit
- Plot predictions will not violate physical limits
e.g. “# of Counts” not negative;
YIELD not > 100%
- Make model more robust
- Make error more uniform across design region
(also called “stabilizing the variance”)
 - Transformations change the scale of the response to make it more nearly conform to the usual regression assumptions, the most important of which are that the data are independent and *follow a normal distribution with a constant variance.*



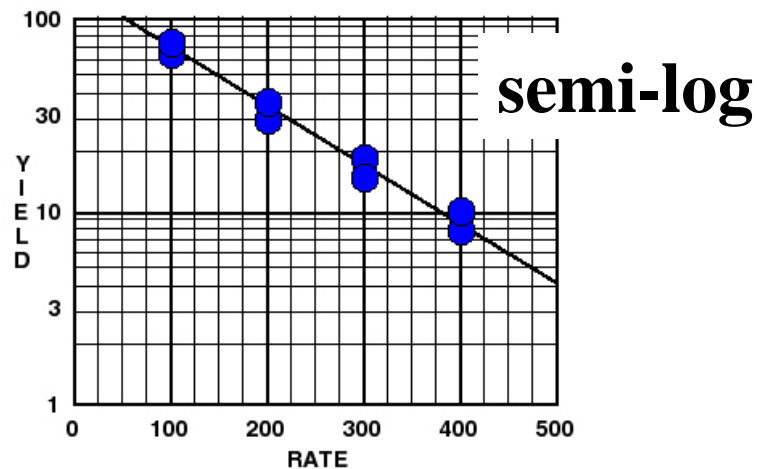
Two Remedies for Lack-of-Fit Fancier *Graph Paper* or Fancier *Curve*



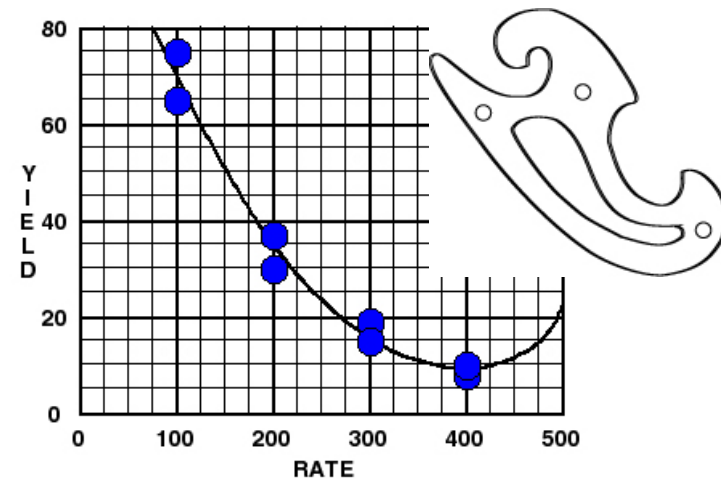
Does not require additional trials.

Usually requires additional trials.

Model Predictions are Virtually Same *within the Range of the Control Variable Settings (100 to 400)*



At Rate = 500
Predicted Yield is 4

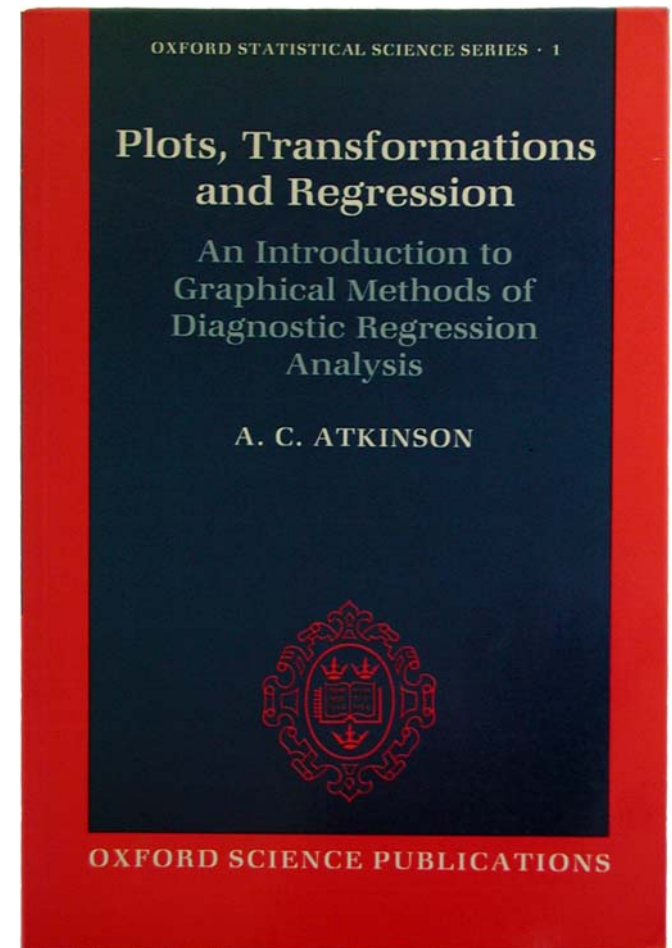


At Rate = 500
Predicted Yield is 22

Which prediction is more suspect? Why?

Have a *Reason* to Use a Transformation- DO NOT "Brute Force" Eliminate Lack-of-Fit

- Consult a book like →
- Check publications in your field to see how others present the same kind of data.
- Consult your local statistical expert.





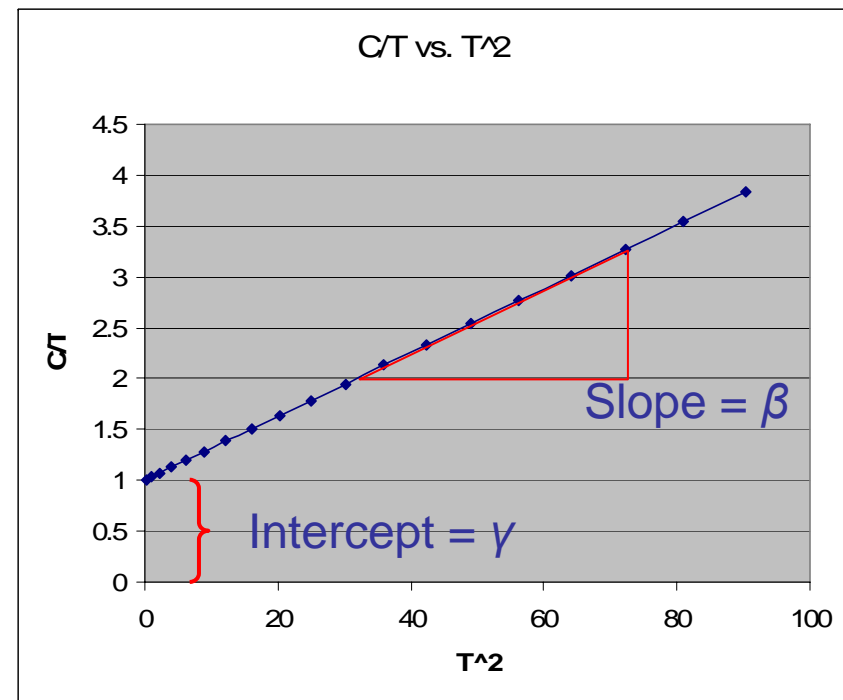
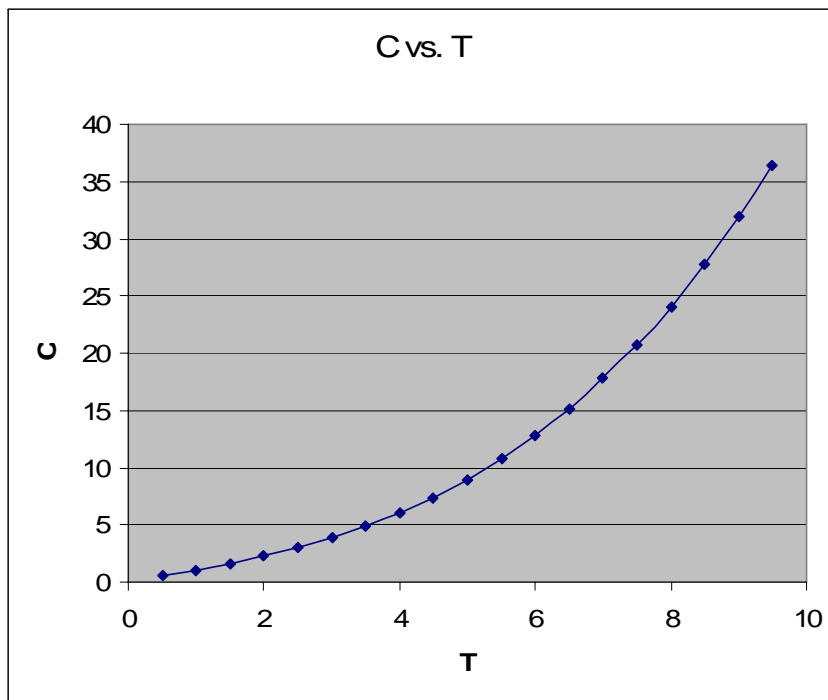
ECS

Example of How Rescaling Makes the Analysis Easier

Specific Heat of Metals for $T < 10^\circ\text{K}$

$$C = \gamma T + \beta T^3$$

$$C/T = \gamma + \beta T^2$$



What Knowledge Did We Use to Choose Variable Scaling?

- Evaporation rate and temperature have an Arrhenius relationship where Evap_Rate is proportional to $e^{(-1/kT)}$ which leads to the scaling choices of taking
 - the \log_{10} of the response, Evaporation Rate, (\log_e could have been used) and
 - the inverse of the control variable Temperature (in °K)
- From Prof. J. Danberg via M. Miller - evaporation rate is proportional to the cube-root of the Wind Velocity
- Believing that evaporation rate was dependent on the area of the drop led to assumption that response should be proportional to square-root of the Drop Size.
 - Recently T. D'Onofrio pointed out that drop size is really a volume and therefore the calculated area of the drops is proportional to $(\text{Drop Size})^{2/3}$. It will be shown that reanalysis of the data using this new scaling makes for very minor changes in predictions and no altering of original conclusions.



Comparison of 10-term Quadratic and 4-term Linear Models

$$\begin{aligned}\log_{10}(y) = & a_0 + a_1x_1 + a_2x_2 + a_3x_3 \\ & + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 \\ & + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2\end{aligned}$$

constant + linear
+ 2-way interactions
+ curvature terms

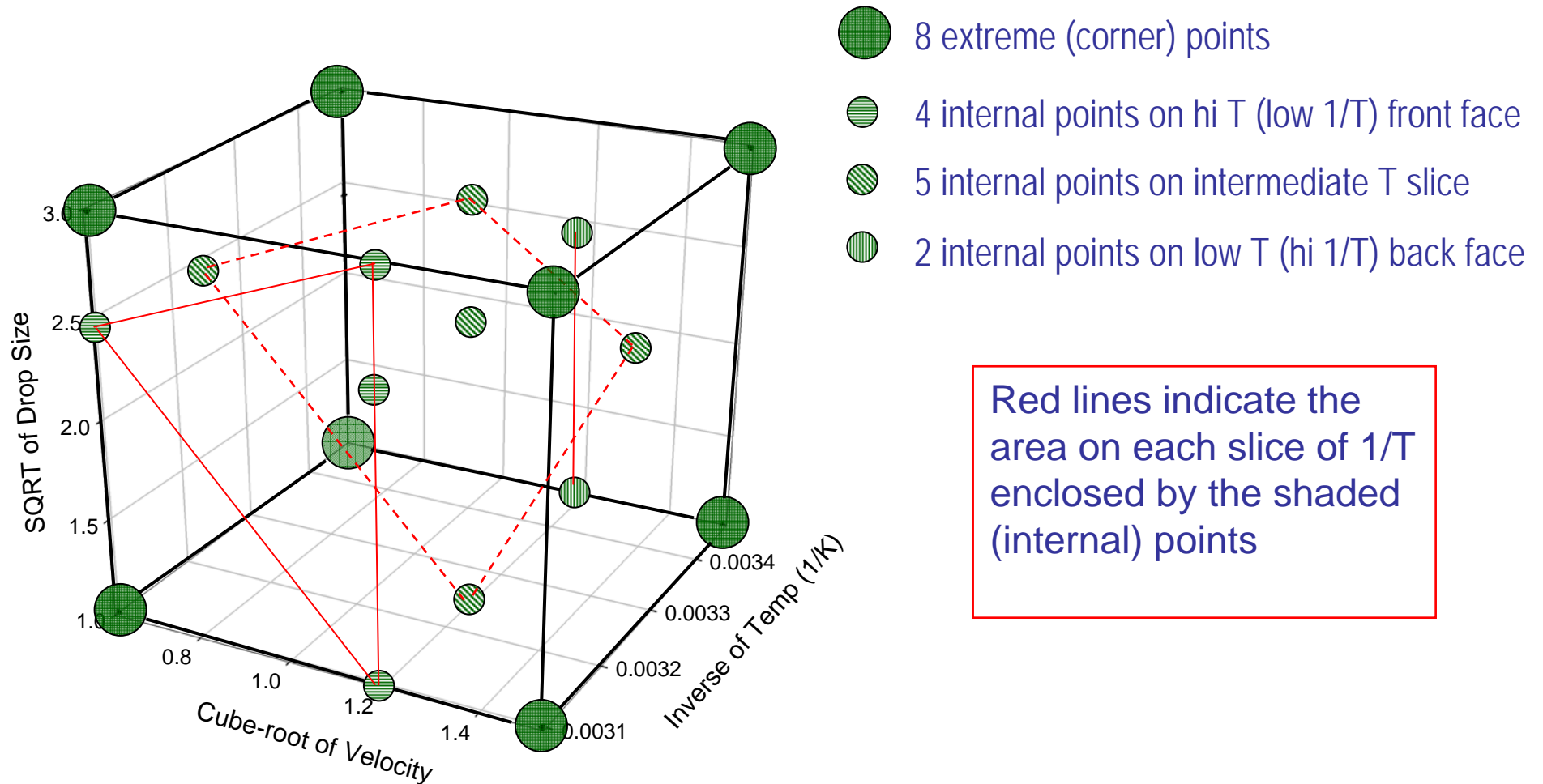
The quadratic model can support many shapes – including; mountain, valley, ridge, saddle and plane.

$$\begin{aligned}\log_{10}(y) = & A_0 + A_1X_1 + A_2X_2 + A_3X_3 \\ \text{and } X_1 = & (x_1)^{-1}, X_2 = (x_2)^{1/2}, X_3 = (x_3)^{1/3}\end{aligned}$$

constant + linear terms
sample exponents used
to “linearize” model

The linear model can only support a plane.

Locations of the 19 Unique Trial Settings for the 5-cm Tunnel

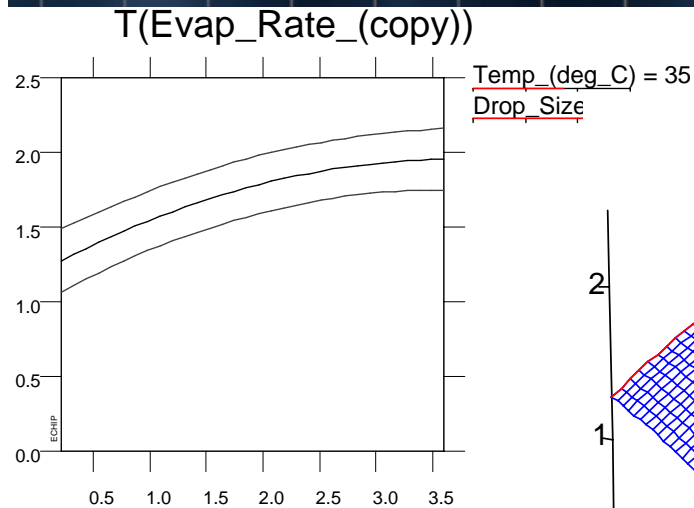




Comments on 5-cm Tunnel Analyses

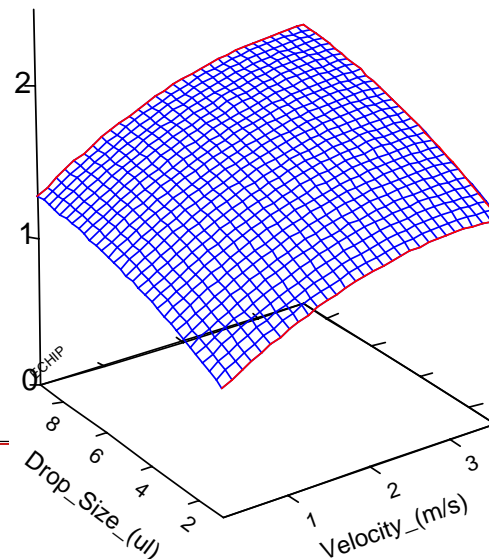
- Good news: Physics-based linearized model fits well - has slightly smaller model error (residual std. dev.) and higher Adjusted-R² than empirical model
- Better news: *Interpolated* model predictions based on fitting data at 8 corner design points are validated by data at locations of 11 interior design trials - which were not used in fitting model
- Even better news: Reversing the situation, the *extrapolated* model predictions based on fitting data at 11 interior points are validated by data at 8 corners - which were not used in fitting model
- Maybe best news: As few as 4 corner points + 1 center point are needed for the 80% solution...

Interpolation with Empirical Quadratic Model (Response Transformed to \log_{10} Scale)

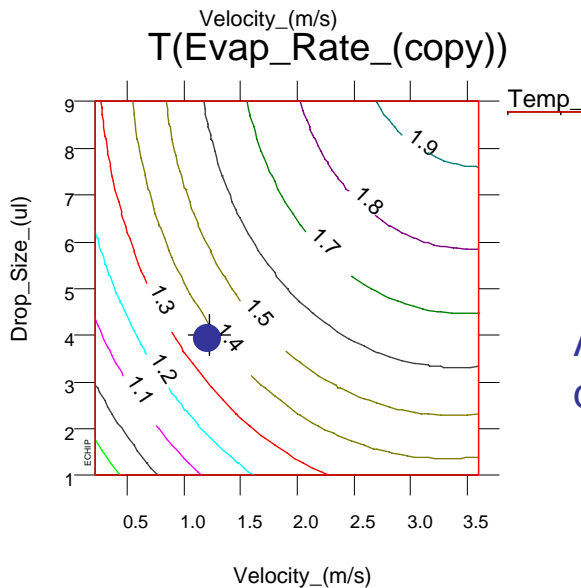


T(Evap_Rate_(copy))

Temp_(deg_C) = 35.0



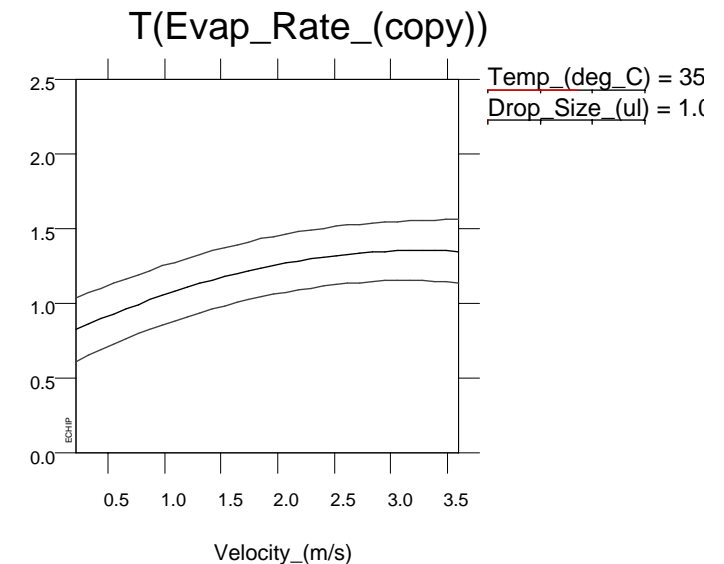
1-D, 2-D & 3-D plots of Evap_Rate
vs. Velocity and Drop_Size
with \log_{10} transformation “applied”



All 19 trials fit using a 10-term
quadratic model

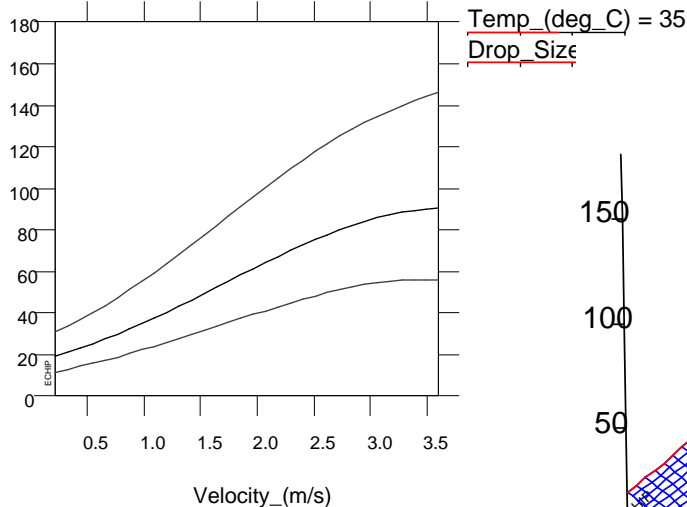
$$10^{1.38} = 24.0$$

Velocity=1.23		Drop_Size=4.00
Value	Plot SD	Predicted SD
1.38	0.04	0.09



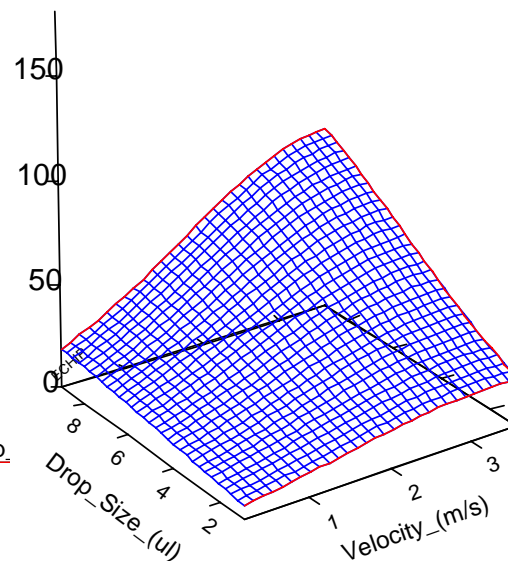
Interpolation with Empirical Model (Response Transformed Back to Original Scale)

Evap_Rate_(copy)



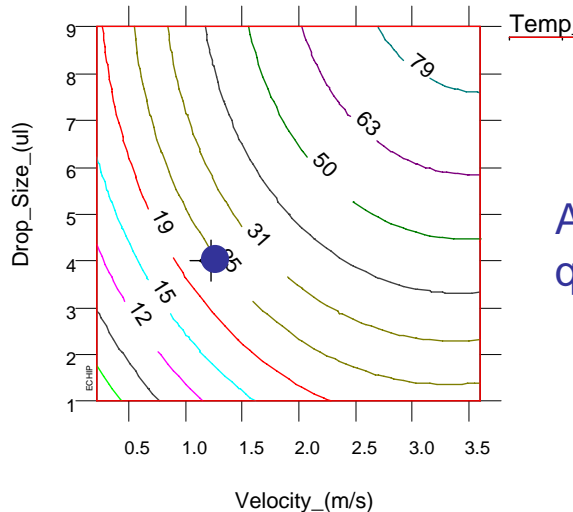
Evap_Rate_(copy)

Temp_(deg_C) = 35.0



1-D, 2-D & 3-D plots of Evap_Rate
vs. Velocity and Drop_Size
with Log₁₀ transformation “undone”

Evap_Rate_(copy)

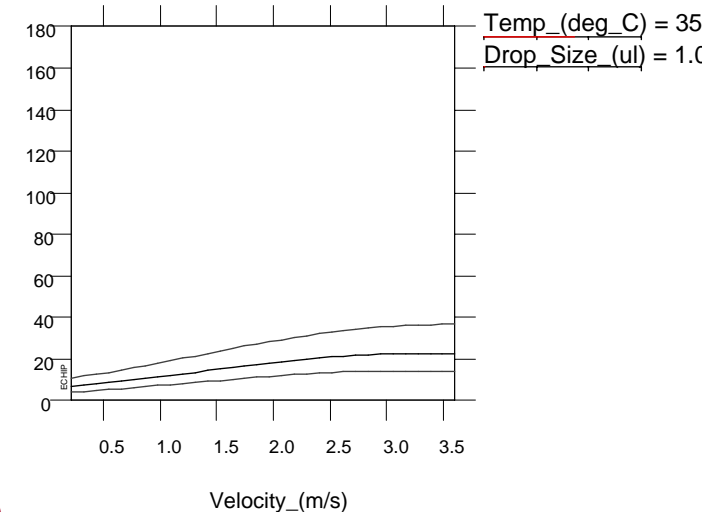


All 19 trials fit using a 10-term
quadratic model

24.2 (15.8, 37.0)

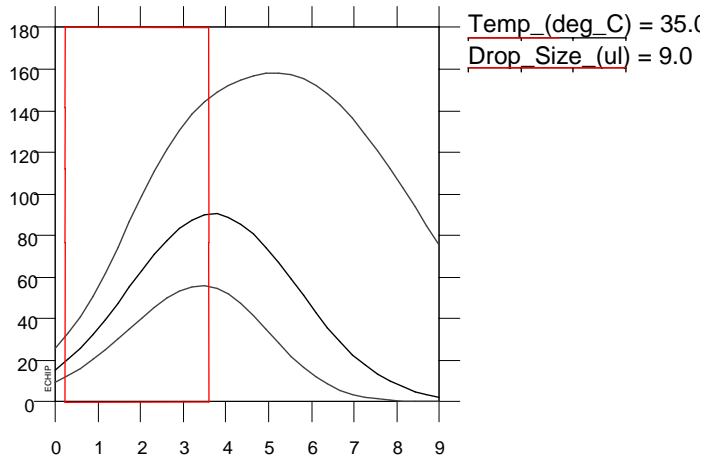
Velocity=1.23	Drop_Size=4.00
Value	Low Limit
24.21	15.83
	High Limit
	37.03

Evap_Rate_(copy)

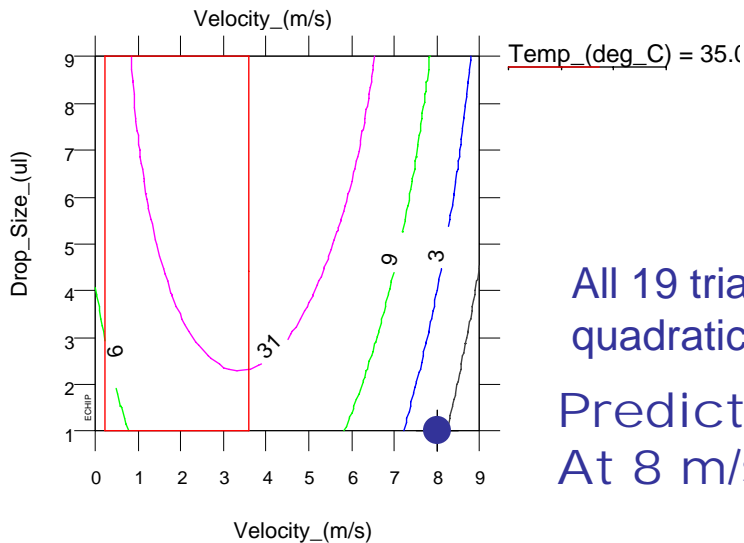
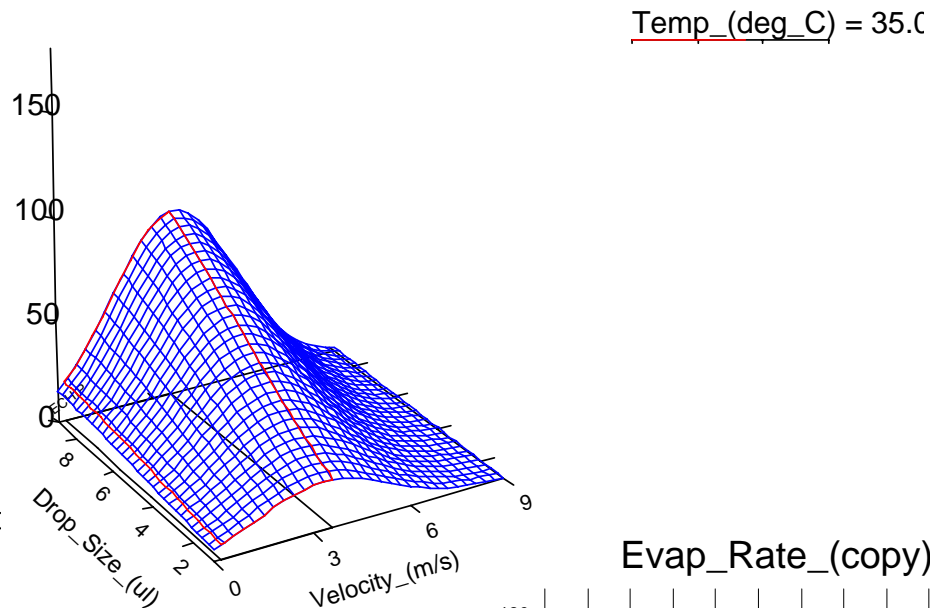


Extrapolation with Empirical Model (Response Transformed Back to Original Scale)

Evap_Rate_(copy)



Evap_Rate_(copy)

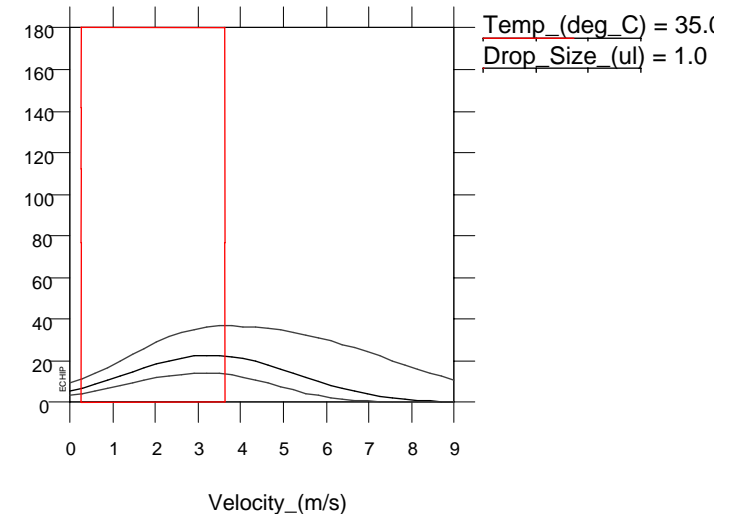


All 19 trials fit using a 10-term
quadratic model

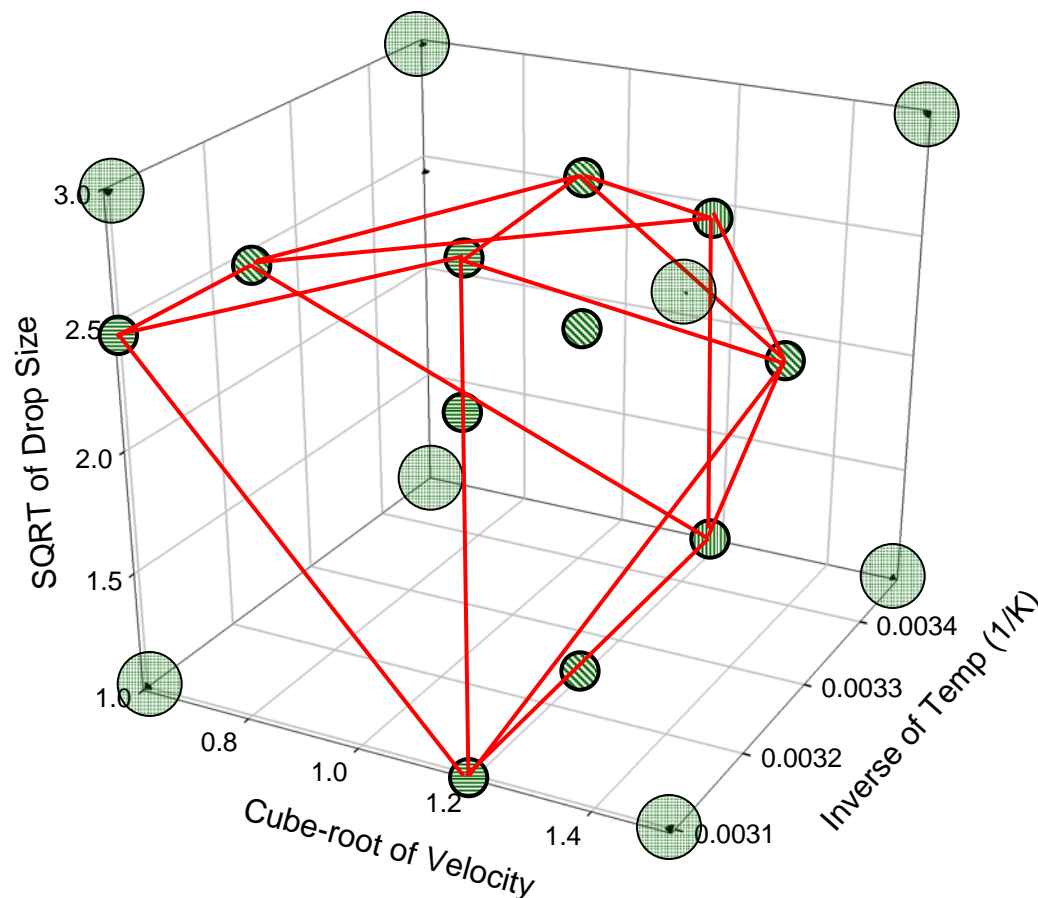
Predicted Evap_Rate
At 8 m/s = 1.3 (0.1, 17.1)

Velocity=8.00	Drop_Siz=1.00
Value	Low Limit
1.33	0.10
	High Limit
	17.11

Evap_Rate_(copy)



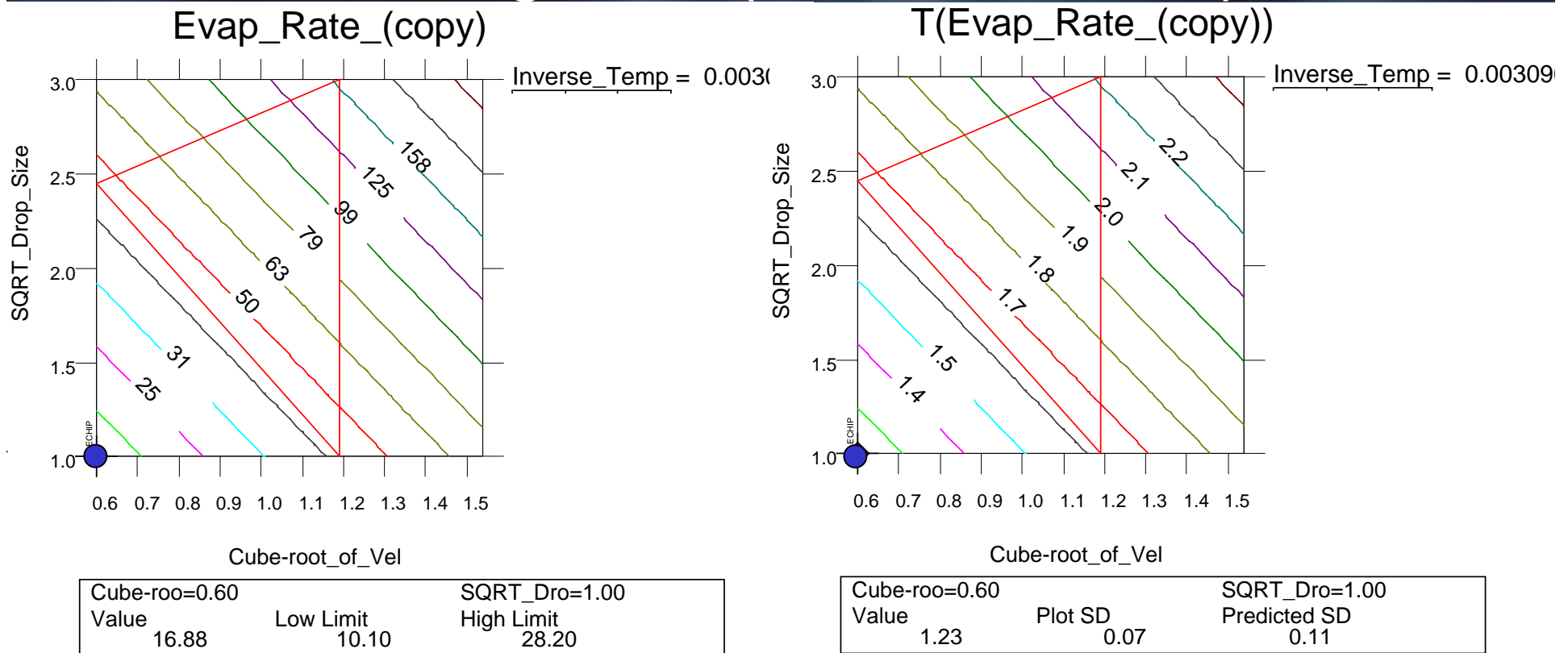
Volume Enclosed by the 11 Unique Interior Trials for the 5-cm Tunnel



The red polyhedral shape results from “shrink wrapping” the 11 non-corner design trials for the 5-cm tunnel.

Predictions at the 8 corners of the design region made using a model fit to these 11 points are *extrapolated* predictions.

Predictions on Raw and Transformed Scales at Location of the Poorest Performing Extrapolated Checkpoint



Predicted value is 16.88 on raw scale
 with 95% Prediction Limits of 10.10 to 28.20
 Observed value was **21.6** on raw scale

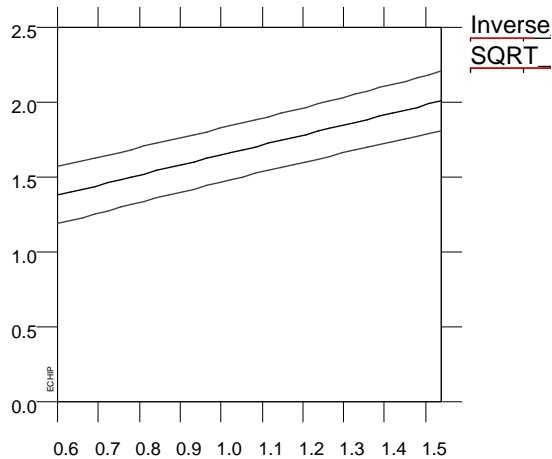
$$\text{Observed Log}_{10}(21.6) = 1.33$$

Predicted value is 1.23 on log10 scale
 Within one Predicted SD (0.11) of the
 Observed value of **1.33** on log10 scale

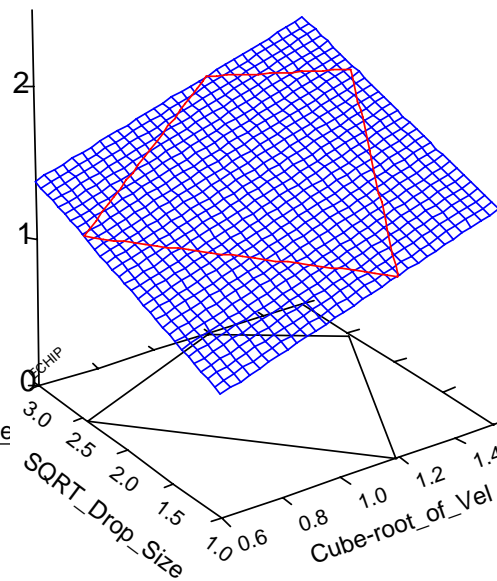
$$\text{Predicted } 10^{1.23} = 16.98$$

Interpolation w/Physics-Based Linear Model (Response Transformed to \log_{10} Scale)

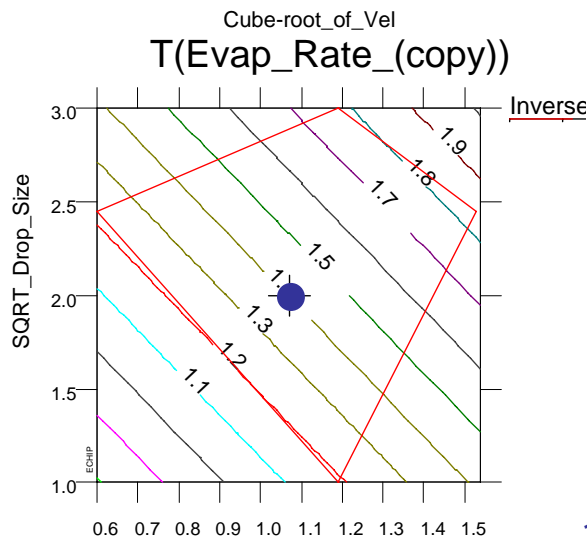
T(Evap_Rate_(copy))



T(Evap_Rate_(copy))

Inverse_Temp = 0.00324

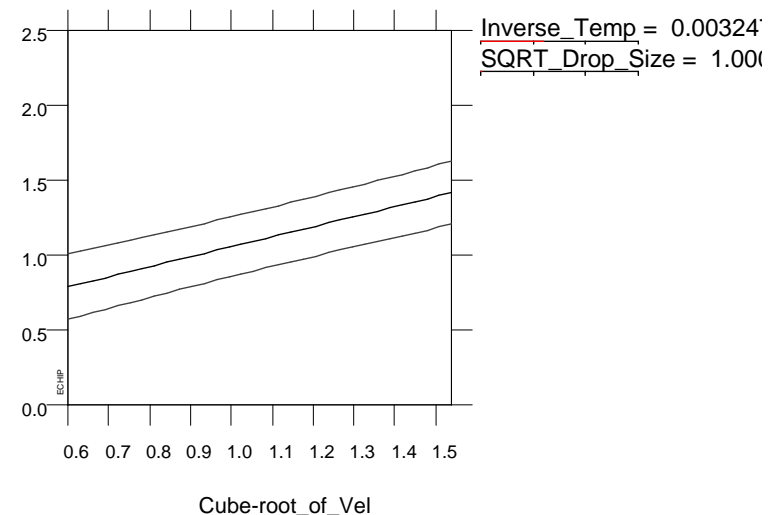
1-D, 2-D & 3-D plots of Evap_Rate vs.
Cube-root_of_Vel & SQRT_Drop_Size
With \log_{10} transformation "applied"



11 interior trials fit using a
4-term linear model that is
physics based

$$10^{1.40} = 25.1$$

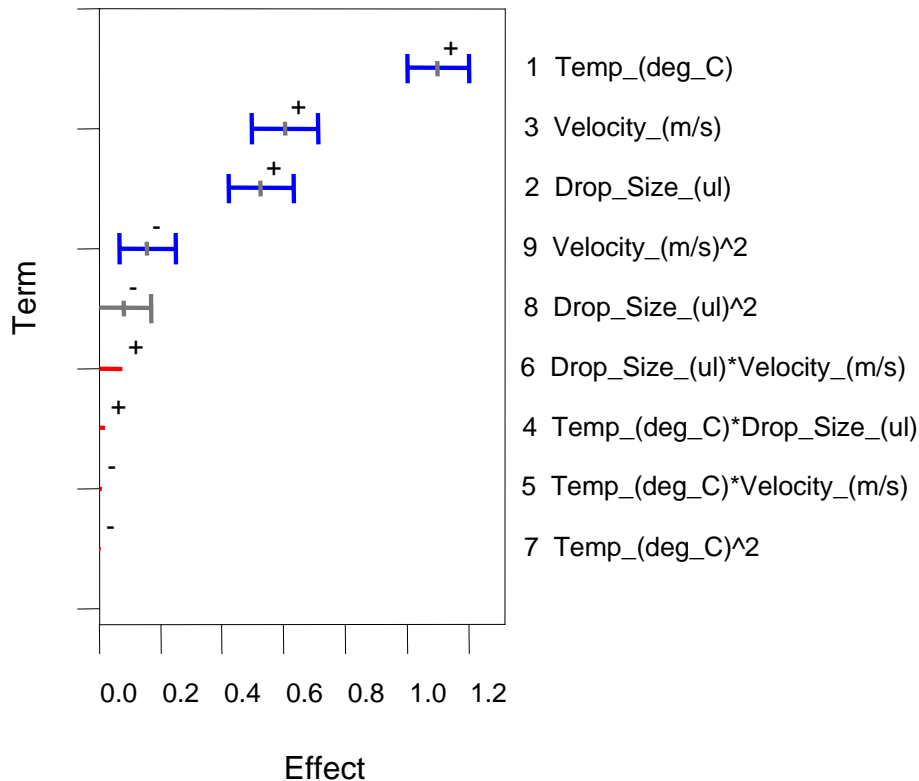
T(Evap_Rate_(copy))



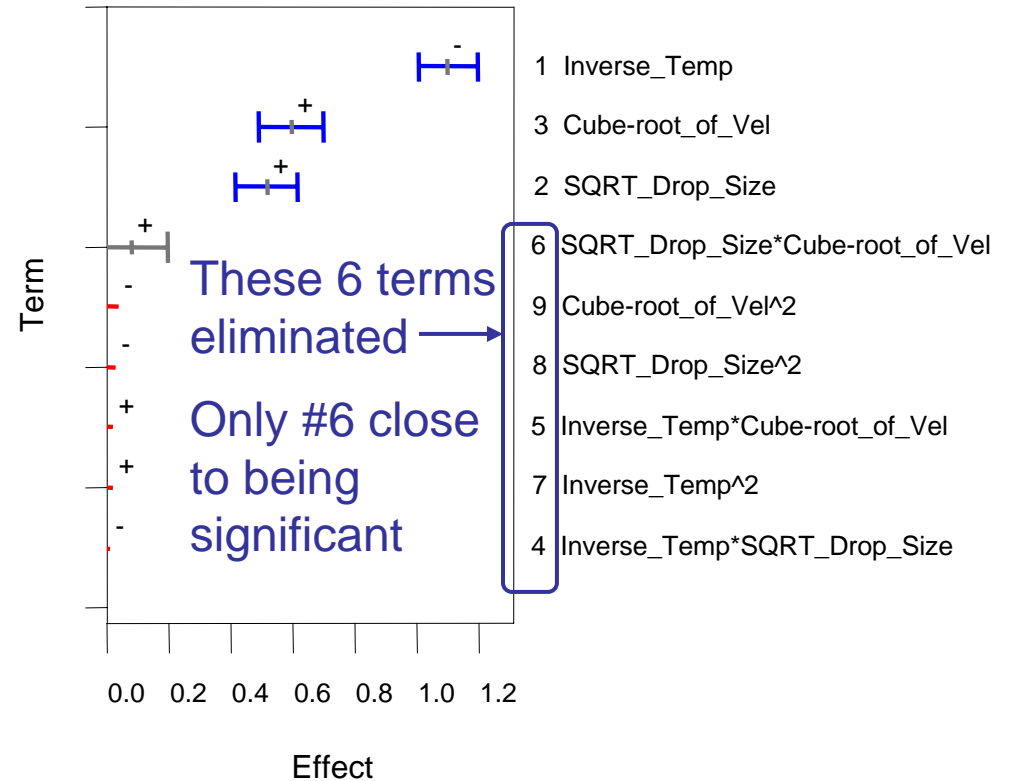
Cube-root=1.07		SQRT_Dro=2.00
Value	Plot SD	Predicted SD
1.40	0.03	0.08

Comparison of Ranked Effect Estimates for 10-term Quadratic Models Fit to Unscaled and Scaled Control Variables

Pareto Effects for $\log_{10}(\text{Evap_Rate})$



Pareto Effects for $\log_{10}(\text{Evap_Rate})$



An Effect is the Change in the Response, $\log_{10}(\text{Evap_Rate})$, Resulting from Changing a Variable Setting from Low to High



Comparison of Model Error Estimates

Quadratic Model without rescaling of control variables

N trials = 19
 N terms = 10
 Residual DF = 9
 Residual SD = 0.0782

Cross val RMS = 0.1061

R Squared = 0.992
 Adj R Squared = 0.983

Linear Model with rescaling of control variables

N trials = 19
 N terms = 4
 Residual DF = 15
 Residual SD = 0.0700 ← **Smaller**

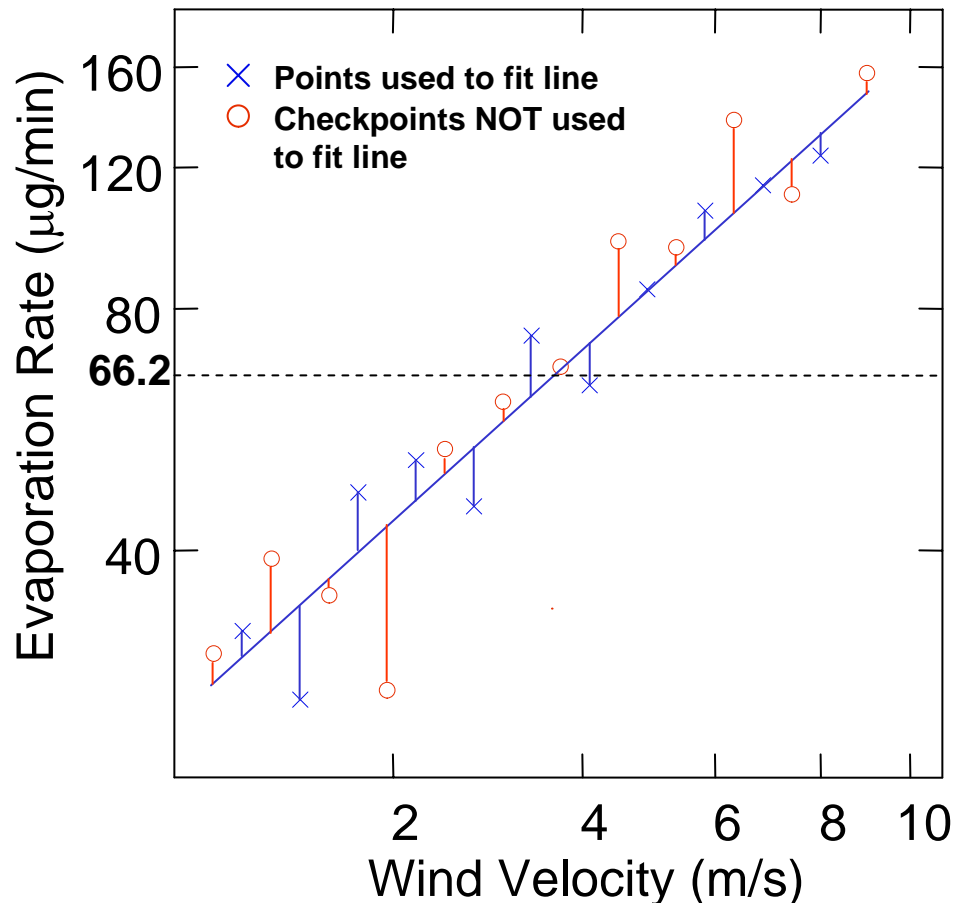
Cross val RMS = 0.0778 ← **Smaller**

R Squared = 0.989
 Adj R Squared = 0.986 ← **Higher**

Results are similar but slightly
 better for the 4-term linear model



Comparing Residual SD, Checkpoint RMS and Raw SD for a Single Control Variable (NOTE: Real Data NOT Used in this Comparison)



N trials = 11
 N terms = 2
 Residual DF = 9
 Residual SD = 0.0655
 (Model error)

N checkpoints = 12
 Checkpoint RMS = 0.0808
 (Prediction error)

Raw SD = 0.2245
 (Error about mean of data
 for 11 trials used to fit)

Graph paper used has \log_{10} vertical scale and cube-root horizontal scale.

Comparing Residual SD, Checkpoint RMS and Raw SD

- When Residual SD ~ Checkpoint RMS then model error is comparable to prediction error
 - Residual SD calculated from the differences between the observed and fitted (predicted) values
 - Checkpoint RMS calculated from the differences between the observed and predicted values - BUT the observed values were NOT used to fit the model used to make the predictions
- Ideally both Residual SD and Checkpoint RMS should be “far” from Raw SD (SD about the Mean of the data)
 - There is no statistical test for how far apart they should be, but for the closer case – the fitting of the 11 internal points - the Raw SD (0.4923) is 6 times larger than both the Checkpoint RMS (0.0765) and the Residual SD (0.0785)



Comparison of Model Error and Checkpoint Error for 8 Corners and 11 Internal Points

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
 N terms = 4
 Residual DF = 4
 Residual SD = 0.0633
 Raw SD = 0.7332

N checkpoints = 11
 Checkpoint RMS = 0.0816
 Cross val RMS = 0.0895

R Squared = 0.996
 Adj R Squared = 0.993

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

N trials = 11
 N terms = 4
 Residual DF = 7
 Residual SD = 0.0785
 Raw SD = 0.4923

N checkpoints = 8
 Checkpoint RMS = 0.0765
 Cross val RMS = 0.1067

R Squared = 0.982
 Adj R Squared = 0.975

Residual SD and Checkpoint RMS Values Agree Well



Comparison of Checkpoint RMS for $V^{1/3}$ term (left) vs. $V^{2/3}$ term (right)

Fitting 8 Corners w/11 Internal Checkpoints

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
 N terms = 4
 Residual DF = 4
 Residual SD = 0.0633
 Raw SD = 0.7332

N checkpoints = 11
Checkpoint RMS = 0.0816
 Cross val RMS = 0.0895

R Squared = 0.996
 Adj R Squared = 0.993

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
 N terms = 4
 Residual DF = 4
 Residual SD = 0.0633
 Raw SD = 0.7332

N checkpoints = 11
Checkpoint RMS = 0.1117
 Cross val RMS = 0.0895

R Squared = 0.996
 Adj R Squared = 0.993

Checkpoint RMS Better with $V^{1/3}$ than with $V^{2/3}$



Comparison of Checkpoint RMS for DS^{1/2} term (left) vs. DS^{2/3} term (right) Fitting 11 Internal w/8 Corner Checkpoints

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

N trials = 11
 N terms = 4
 Residual DF = 7
 Residual SD = 0.0785
 Raw SD = 0.4923

N checkpoints = 8
 Checkpoint RMS = 0.0765
 Cross val RMS = 0.1067

R Squared = 0.982
 Adj R Squared = 0.975

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

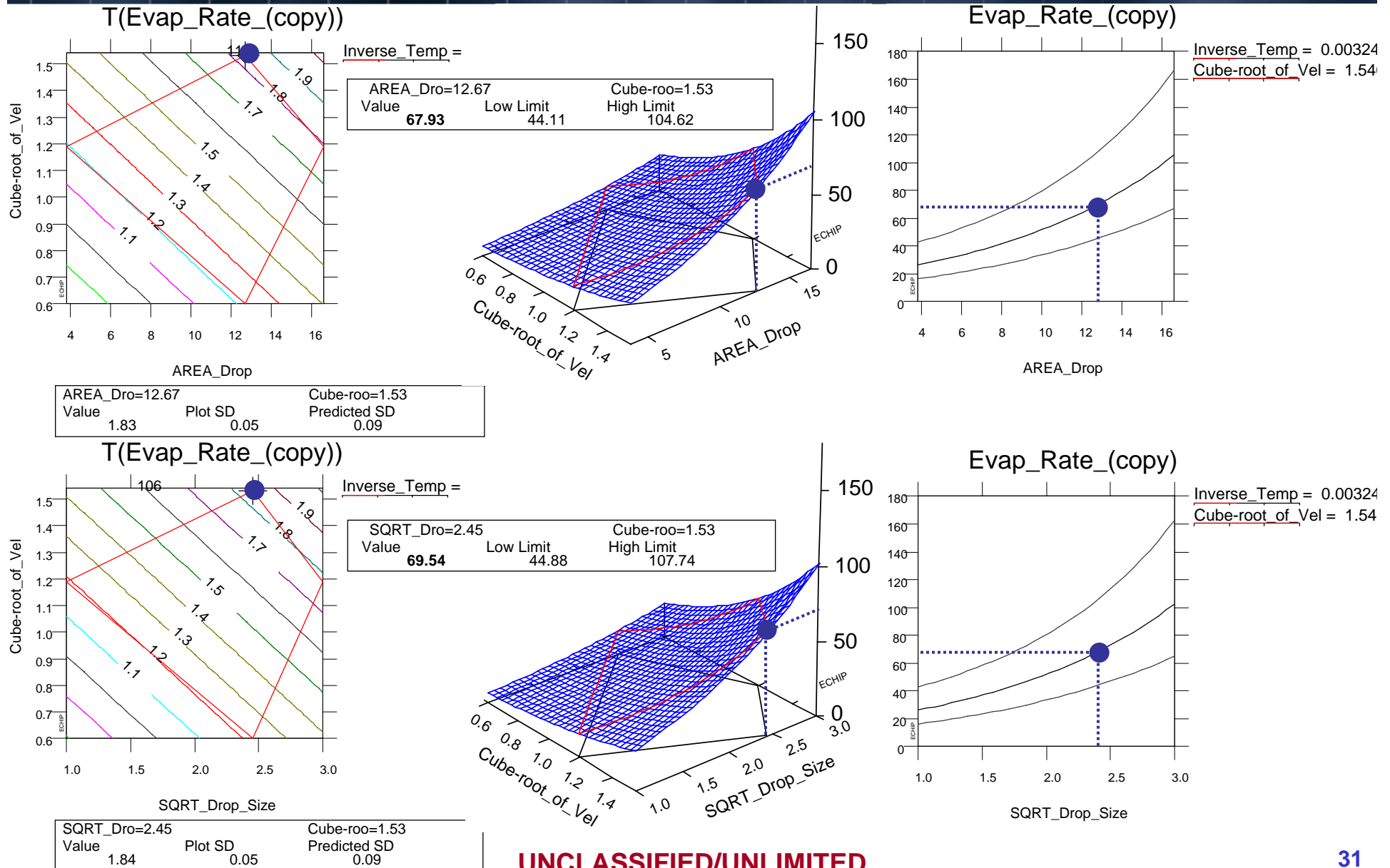
N trials = 11
 N terms = 4
 Residual DF = 7
 Residual SD = 0.0776
 Raw SD = 0.4923

N checkpoints = 8
 Checkpoint RMS = 0.0857
 Cross val RMS = 0.1062

R Squared = 0.983
 Adj R Squared = 0.975

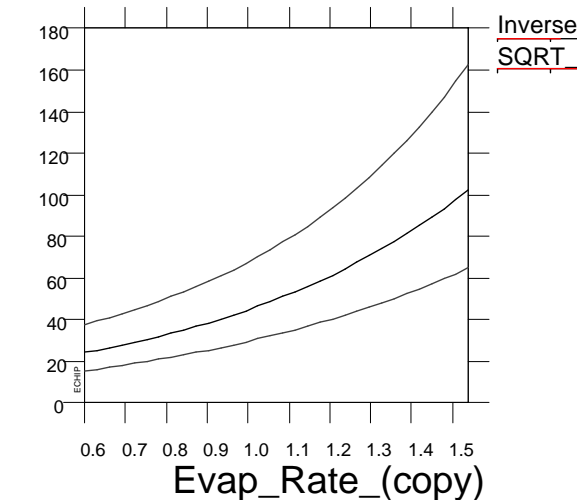
Checkpoint RMS Better with DS^{1/2} than with DS^{2/3}

Compare Predictions for Models Using AREA_Drop vs. SQRT_Drop_Size



Interpolation w/Physics-Based Linear Model (Response Transformed Back to Original Scale)

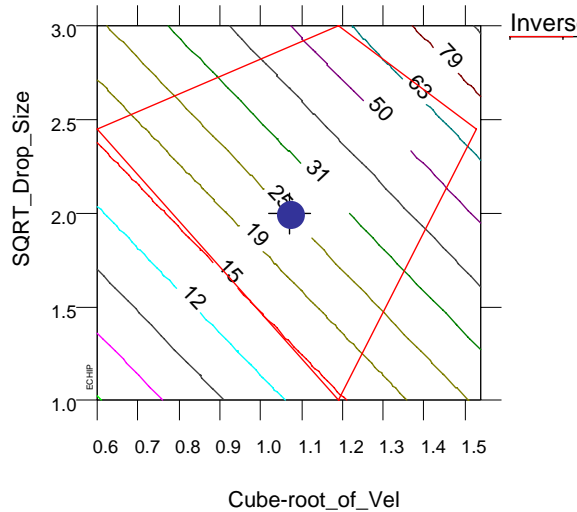
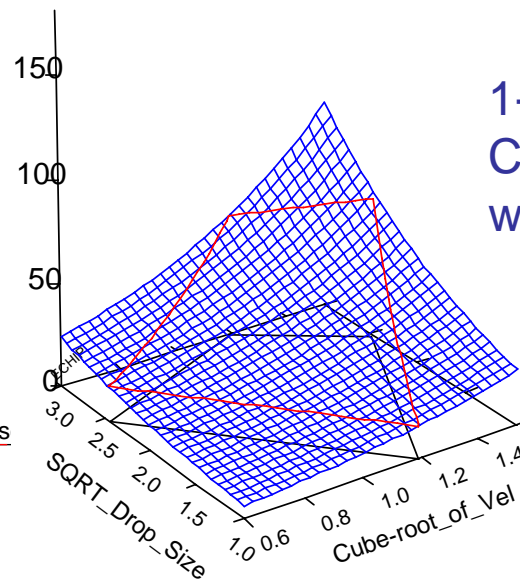
Evap_Rate_(copy)



Evap_Rate_(copy)

Inverse_Temp = 0.00324

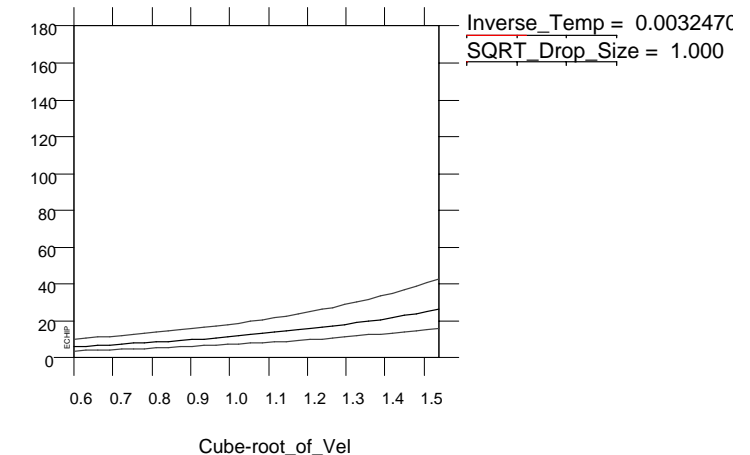
1-D, 2-D & 3-D plots of Evap_Rate vs. Cube-root_of_Vel & SQRT_Drop_Size with Log₁₀ transformation "undone"



11 interior trials fit using a 4-term linear model that is physics based

25.3 (17.0, 37.6)

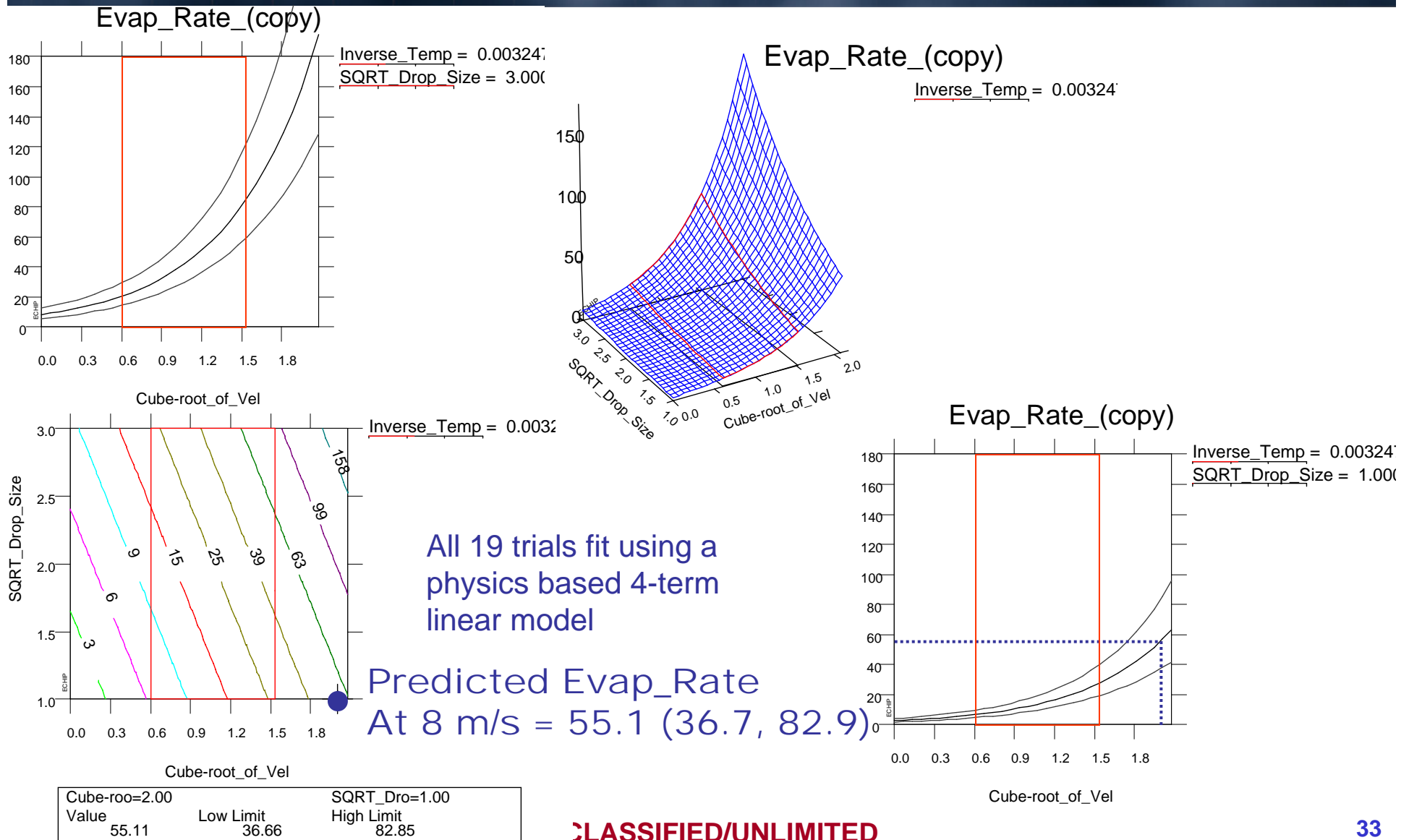
Evap_Rate_(copy)



— Cube-root_of_Vel
- - - Limits

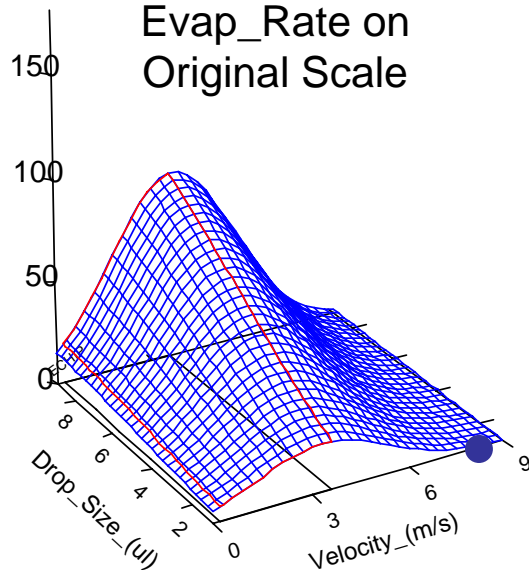
Cube-roo=1.07		SQRT_Dro=2.00
Value	Low Limit	High Limit
25.25	16.97	37.58

Extrapolation with Physics-Based Model (Response Transformed Back to Original Scale)

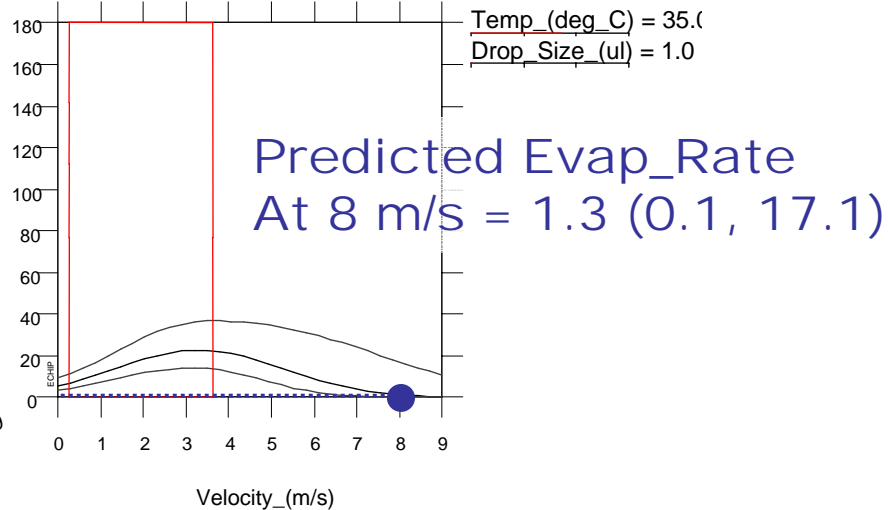


Compare Extrapolations for Empirical (Quadratic) & Physics-Based (Linear) Models (Response Transformed Back to Original Scale)

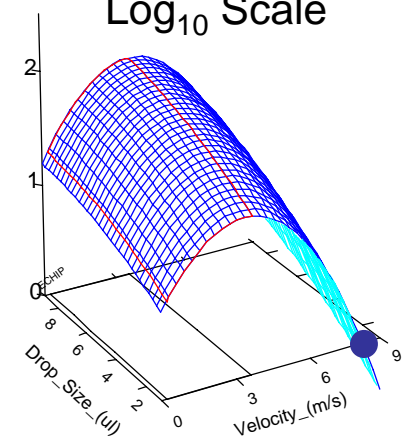
Evap_Rate on Original Scale



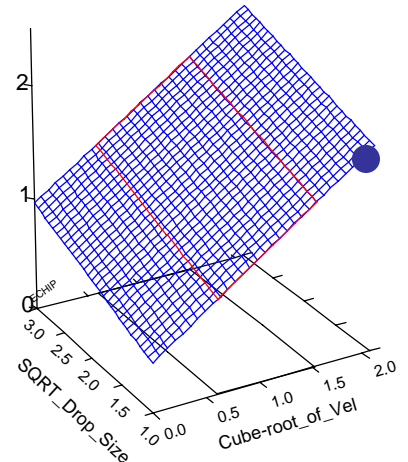
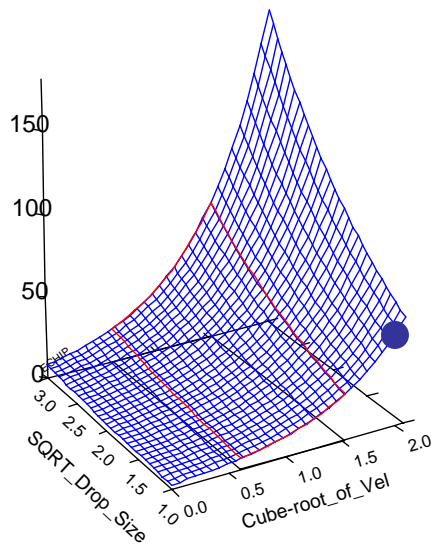
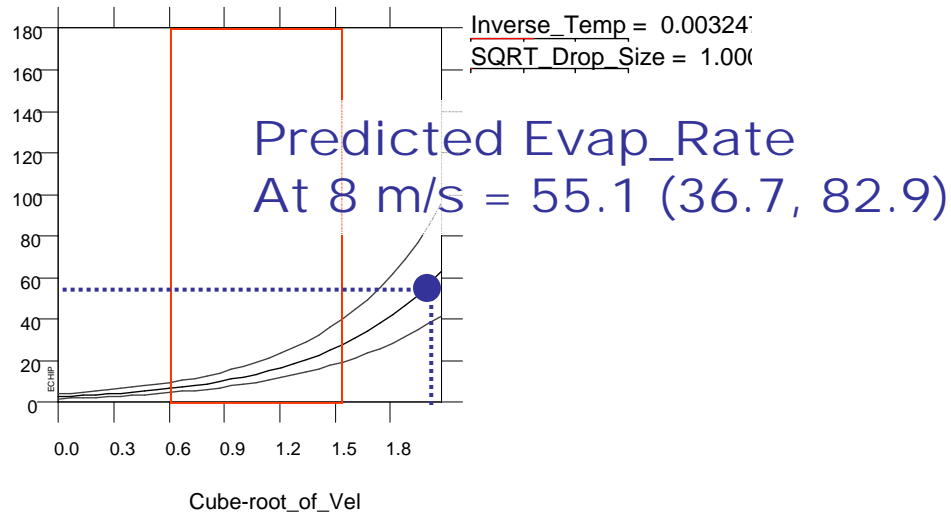
Evap_Rate_(copy)



Evap_Rate on Log₁₀ Scale



Evap_Rate_(copy)



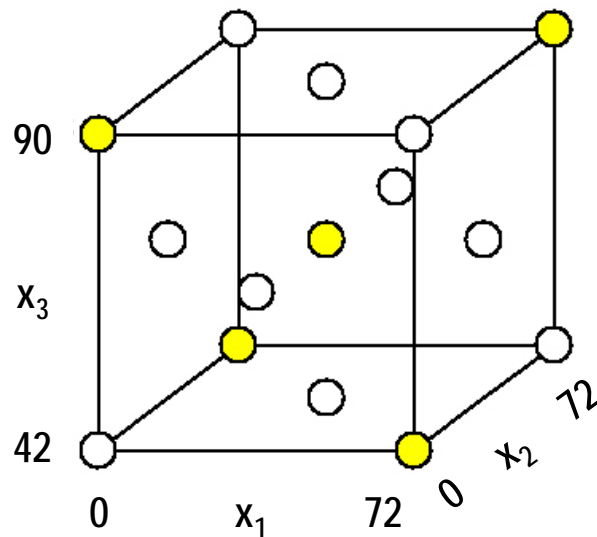
Cube-root_of_Vel

UNCLASSIFIED/UNLIMITED



Sequentially Run Trials in Blocks

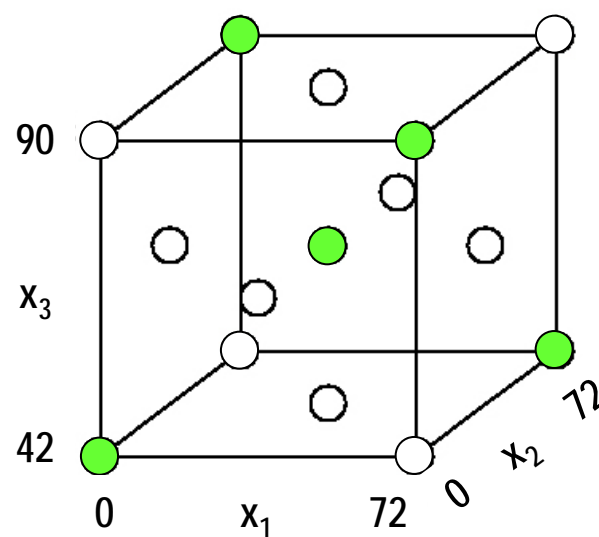
Block 1



$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Linear model is supported by any of the three Blocks

Block 2

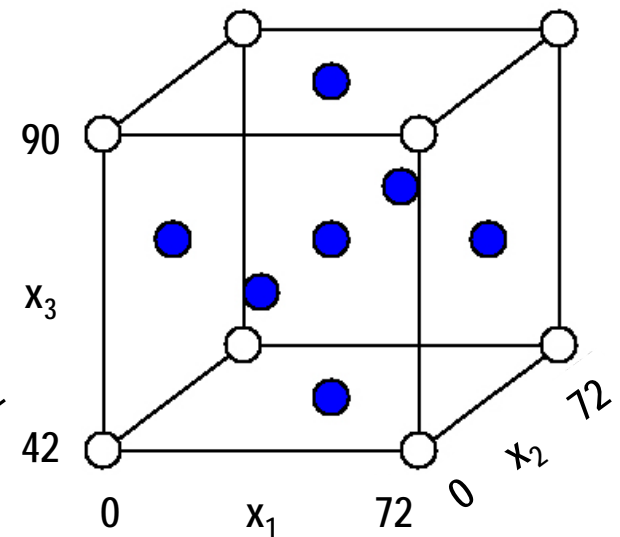


$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

Interaction model is supported by combining first two Blocks

Block 3



$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

$$+ a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$

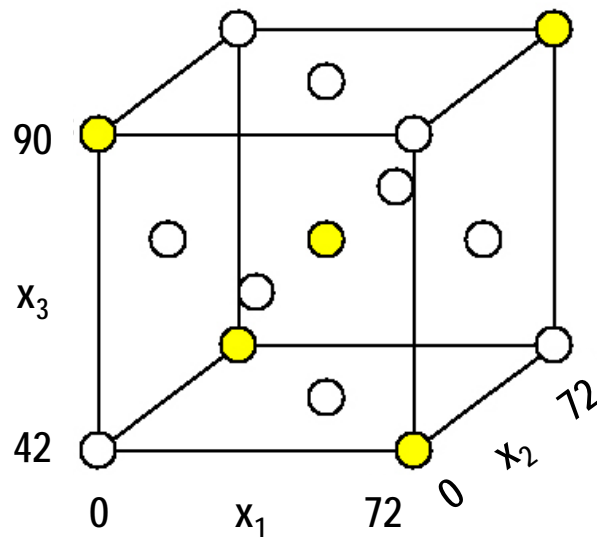
Quadratic model requires all three Blocks to be supported

Blocking is used to prevent correlations between design variables and sources of variation such as unknown variables (e.g. blocks run weeks apart) or differences among groups of trials (e.g. each block associated with a unique “lot” of raw material)



Sequentially Run Trials in Blocks

Block 1

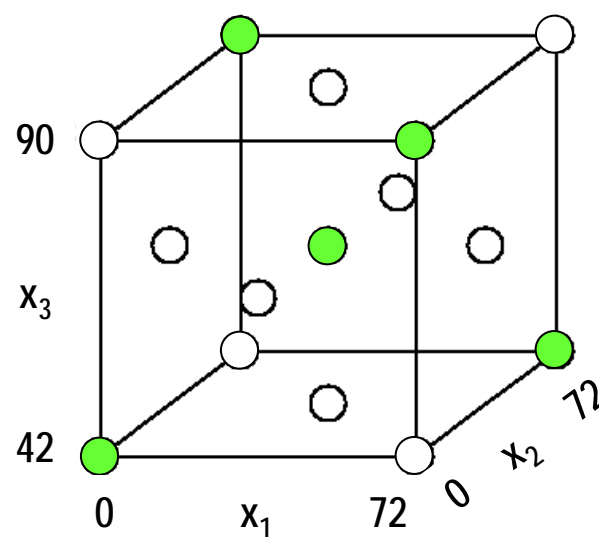


$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Run this block 1st to

- (i) estimate the main effects
- (ii) use center point to check for curvature.

Block 2



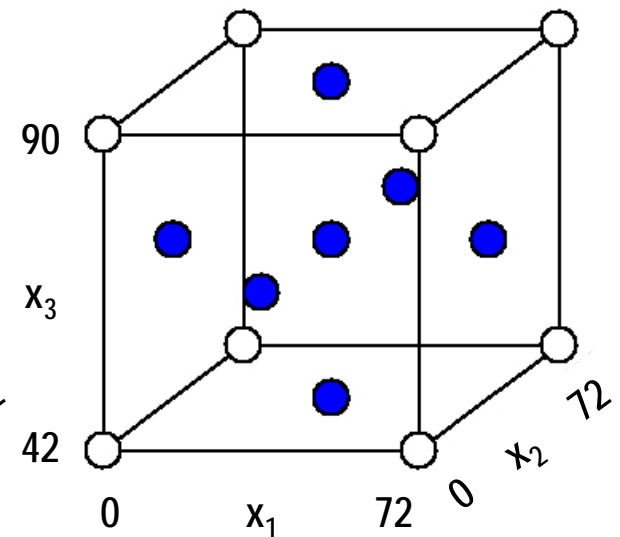
$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

Run this block 2nd to

- (i) repeat main effects estimate,
- (ii) check if process has shifted
- (iii) add interaction effects to model if needed.

Block 3



$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

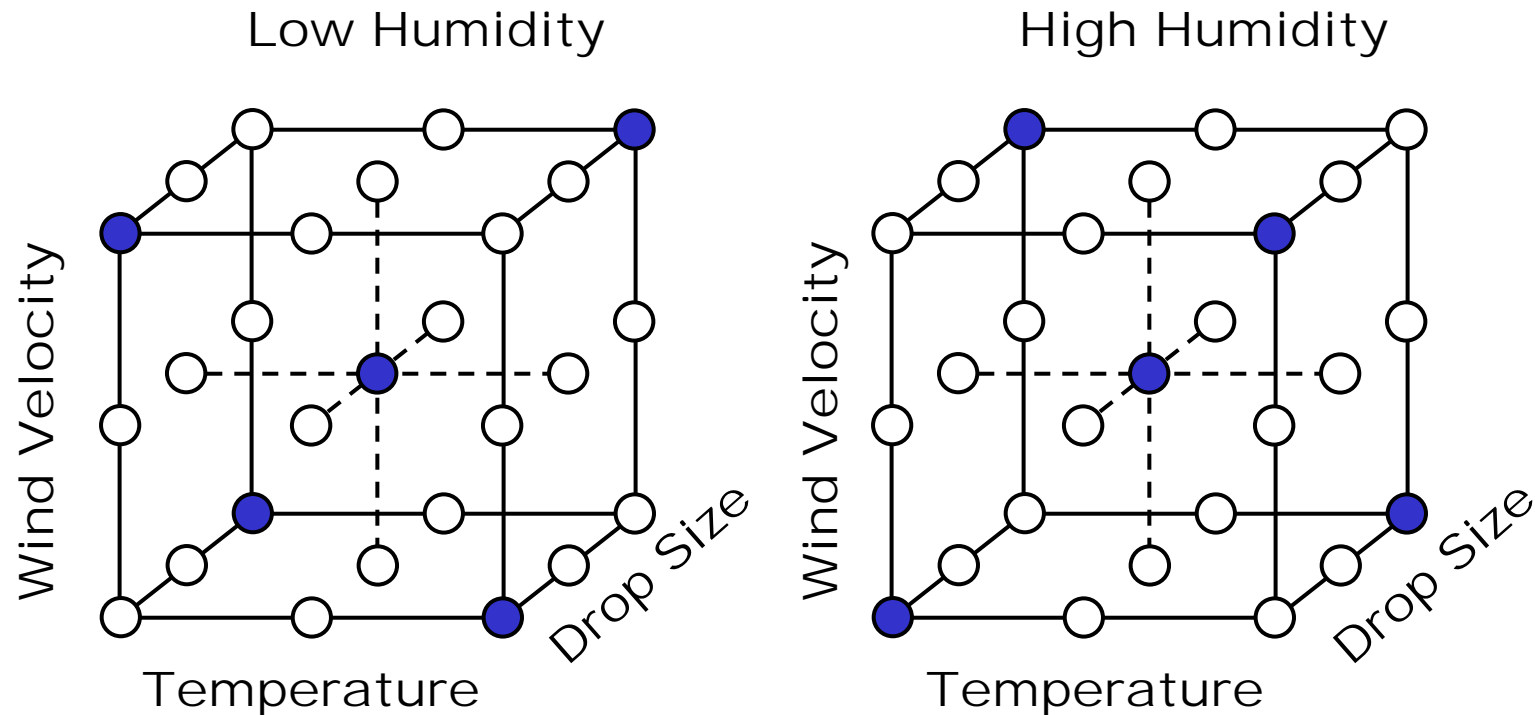
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

$$+ a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$

Run this block 3rd to

- (i) repeat main effects estimate,
- (ii) check if process has shifted
- (iii) add curvature effects to model if needed.

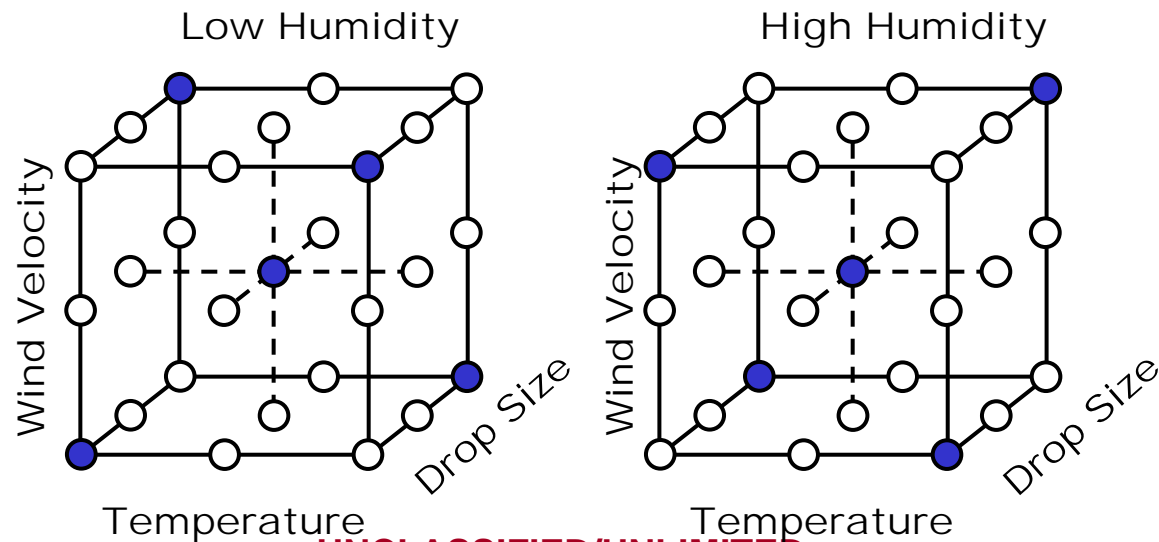
Less than 20% of Originally Planned Trials are Needed to Fit a 5-term Linear Model



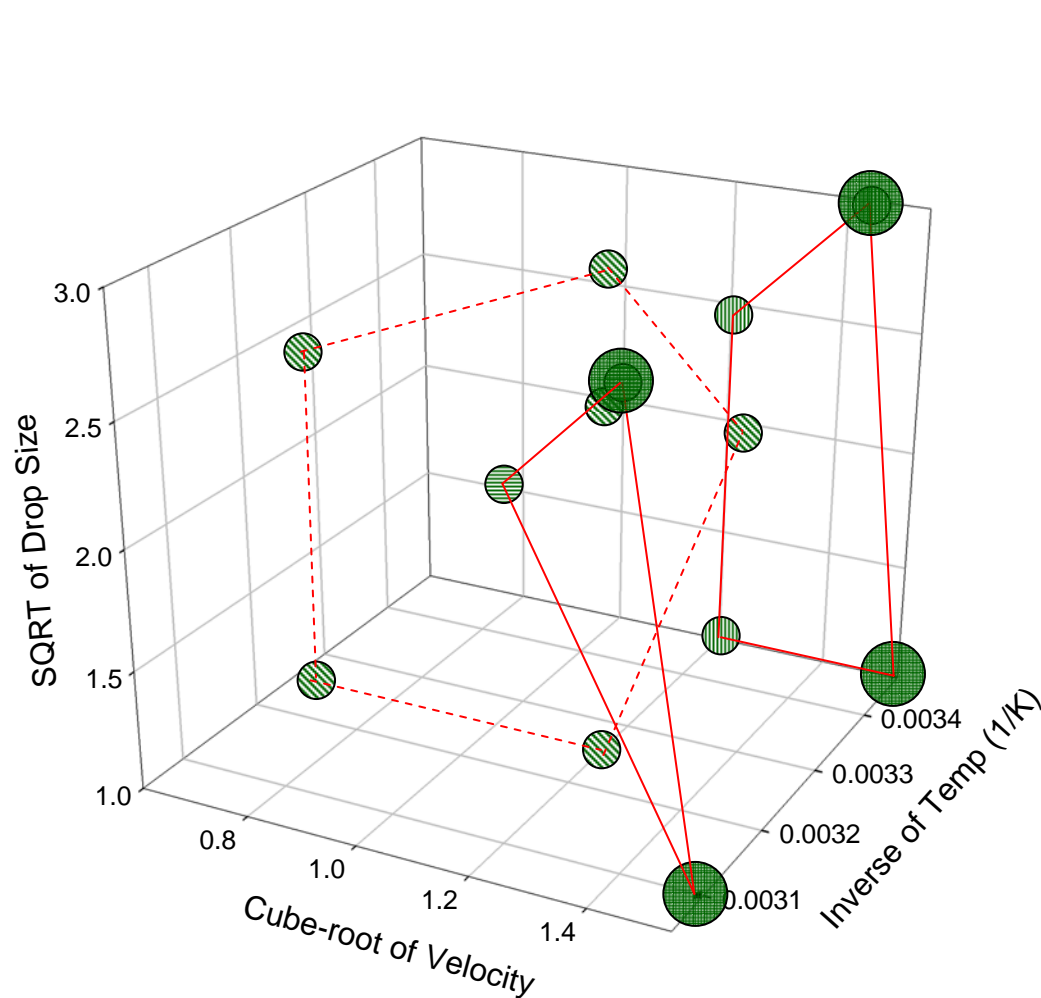
Original plan called for running all $3 \times 3 \times 3 \times 2 = 54$ combinations of settings of Wind Velocity (3 levels), Temperature (3 levels), Drop Size (3 levels) and Humidity (2 levels). The 10 blue locations are all that are needed to estimate the main effects which physics-based scaling of the axes showed well-fit the Evaporation Rate data for HD on glass.

Agents & Substrates other than HD on Glass Will Likely Require More Complex Models

- It still makes sense to acquire data for fitting these models as efficiently as possible.
- Running the trials in randomized blocks of trials will help to facilitate this goal.
- Shown below is a second block that when added to the one on the preceding slide will support the 4 variable 11-term interaction model.



Locations of the 13 Unique Trial Settings for the 10-cm Tunnel



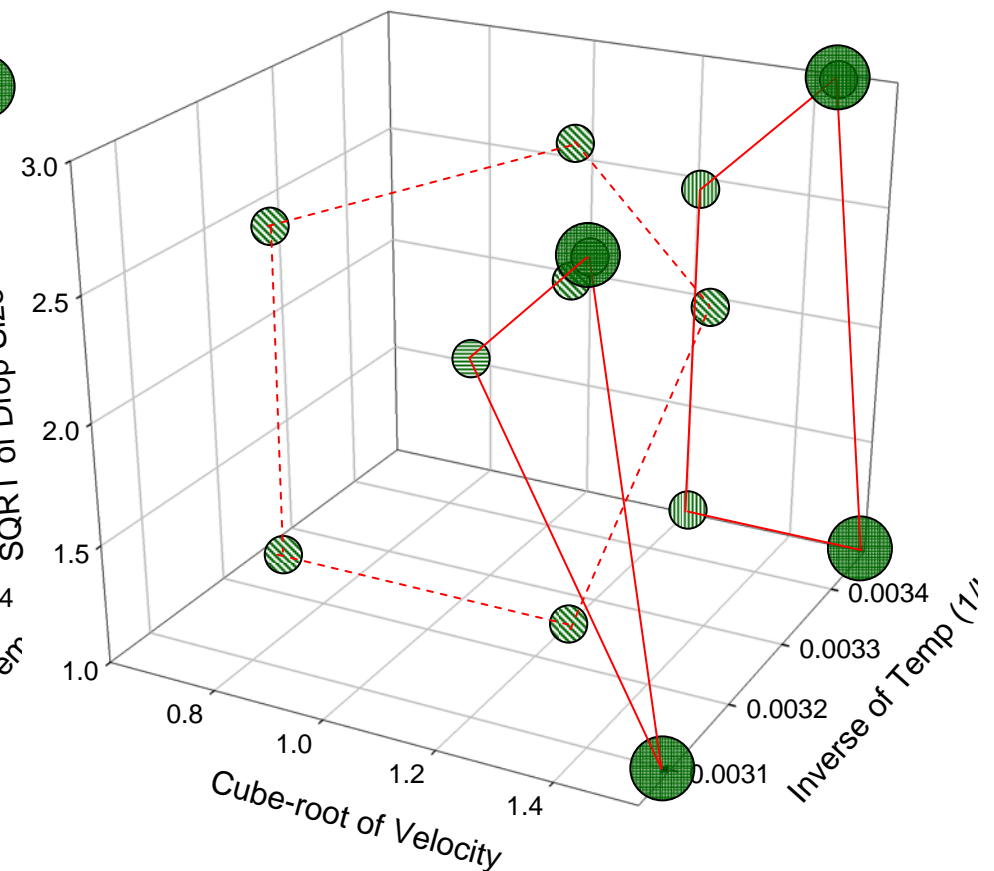
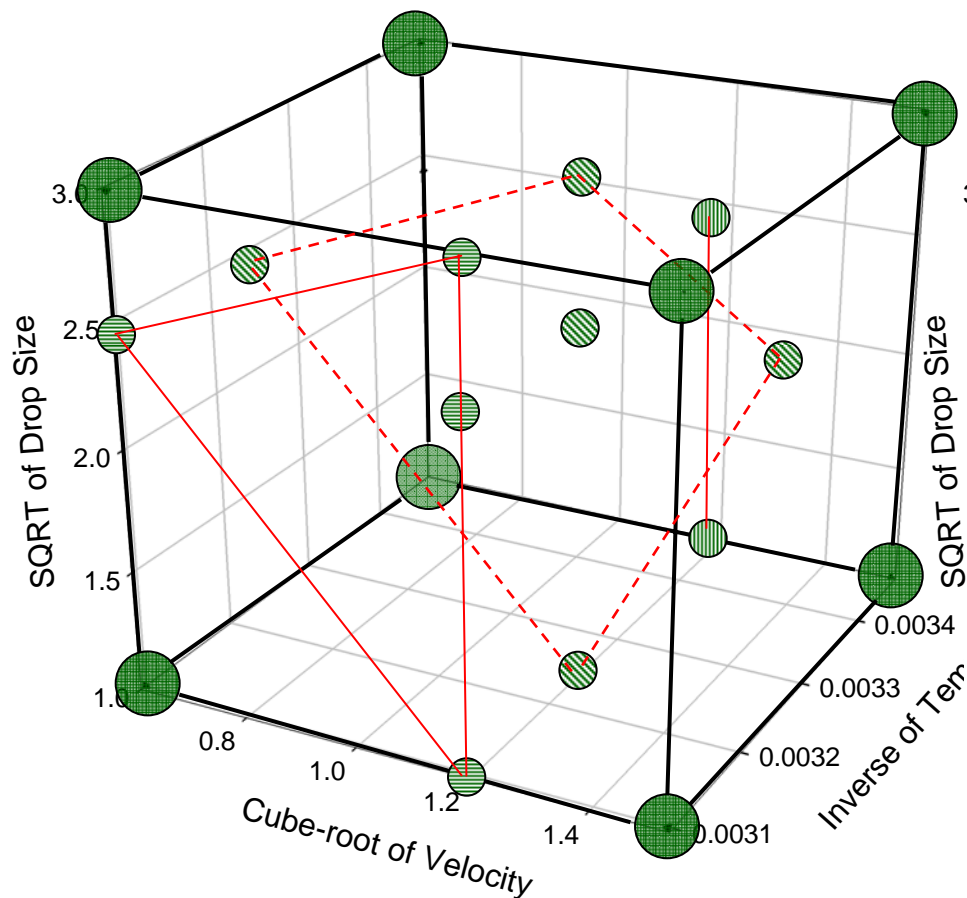
- 4 extreme (corner) points
- 1 internal point on hi T (low 1/T) front face
- 6 internal points on intermediate T slice
- 2 internal points on low T (hi 1/T) back face

Red lines indicate the area on each slice of 1/T enclosed by all points



Locations of the 19
unique trial settings
for the 5-cm tunnel

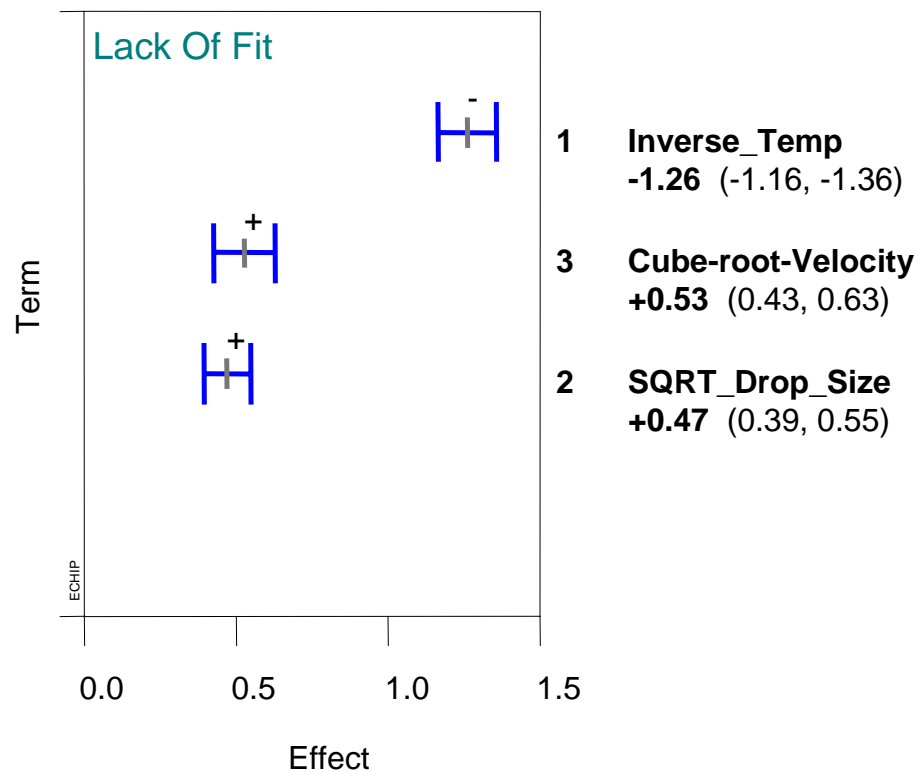
Locations of the 13
unique trial settings
for the 10-cm tunnel



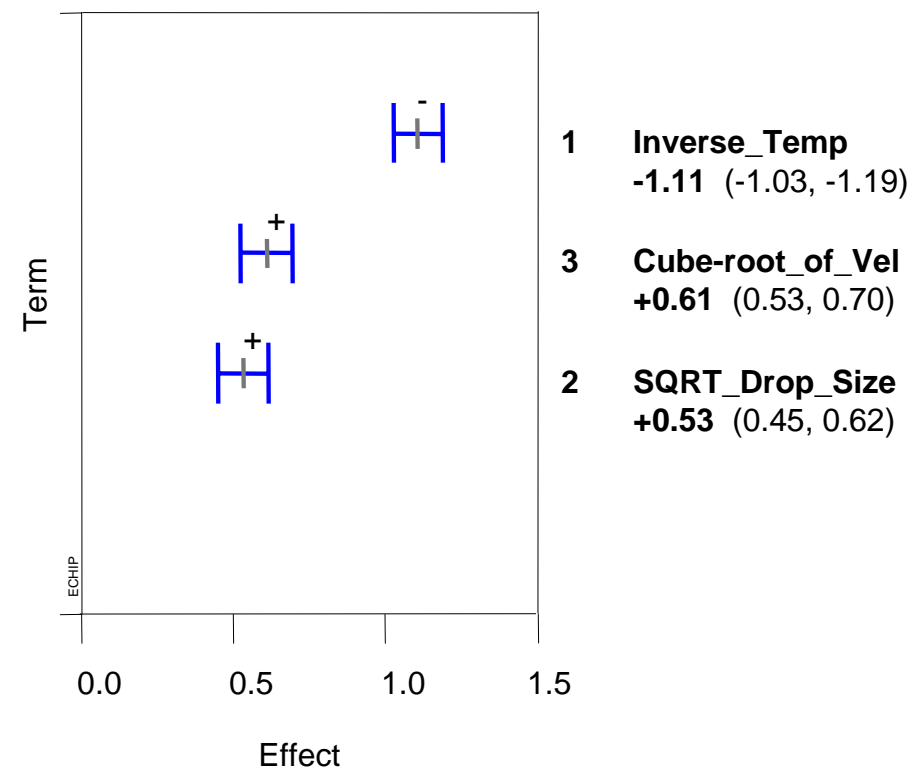
An Effect is the Change in the Response Resulting from Changing a Variable Setting from Low to High

Results for the 2 tunnels are very similar

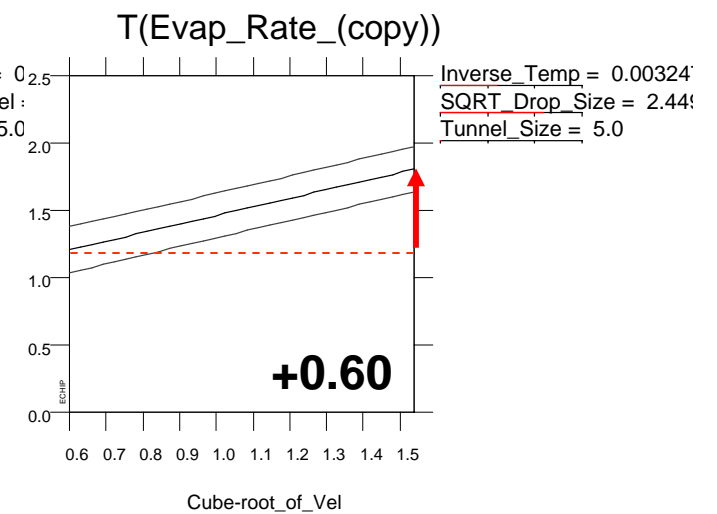
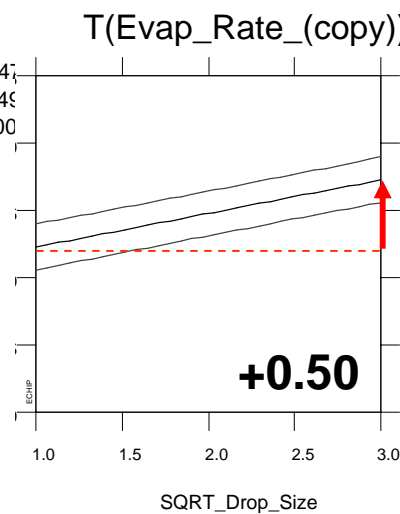
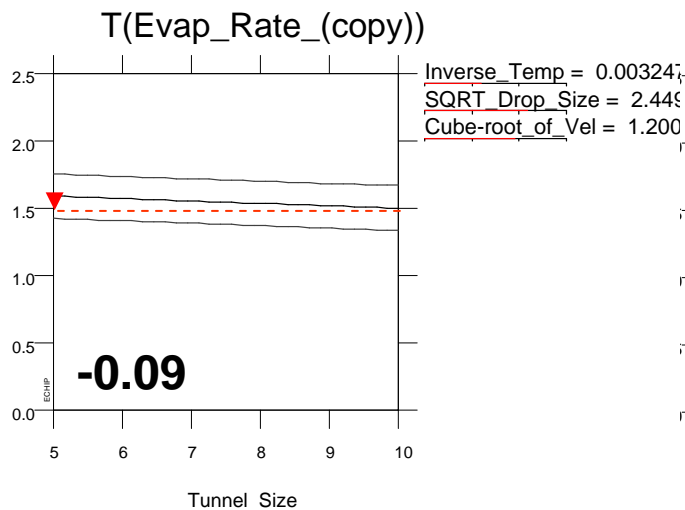
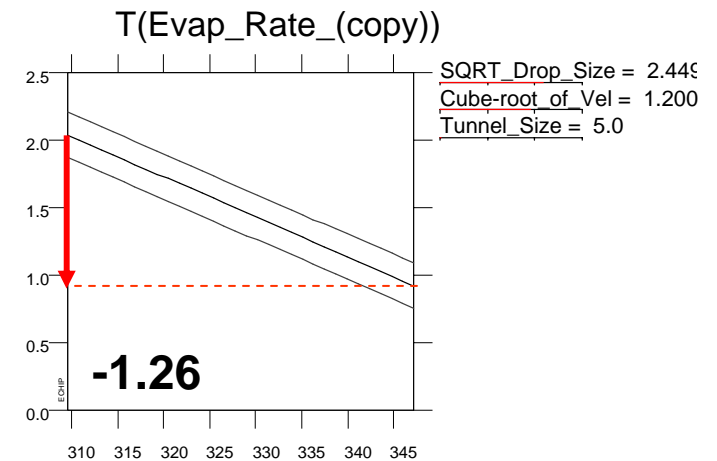
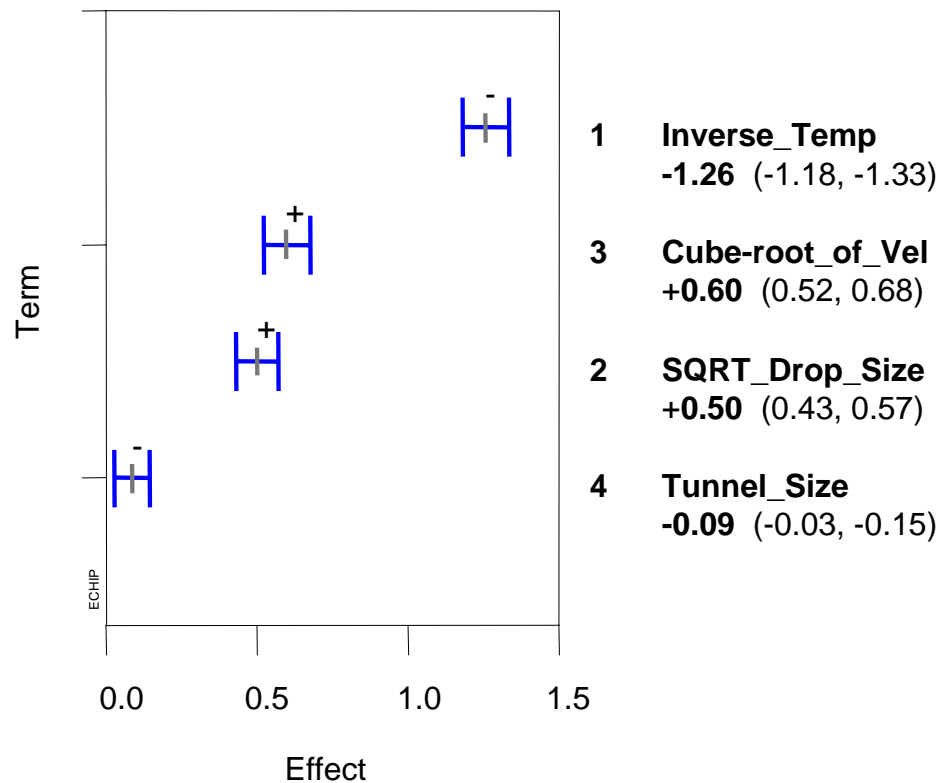
Pareto Effects for
 $\text{Log}_{10}(\text{Evap_Rate})$
10-cm tunnel



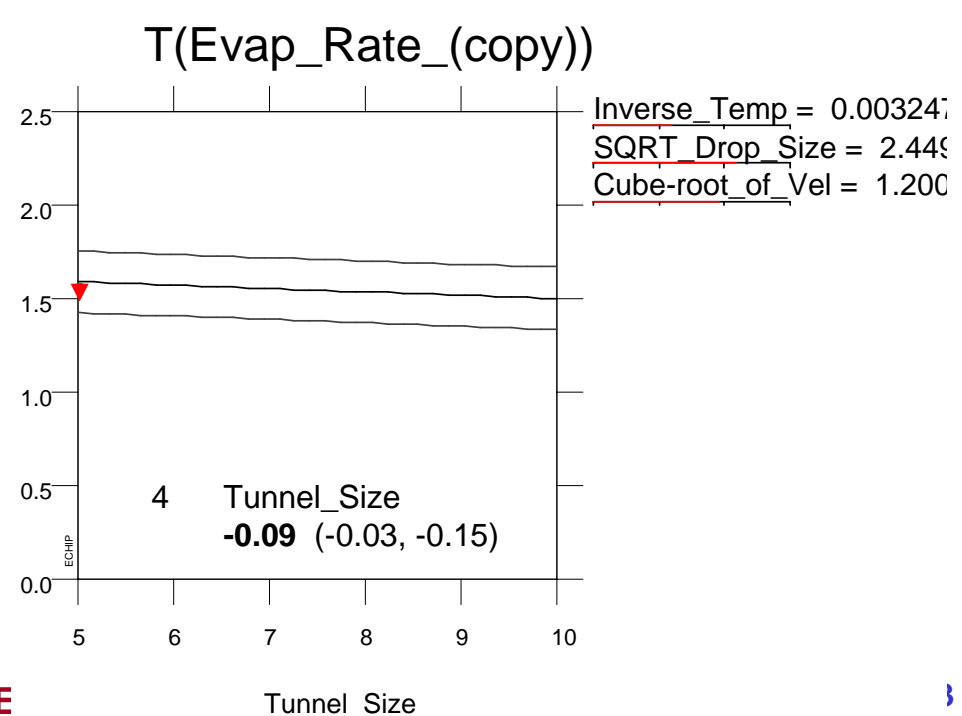
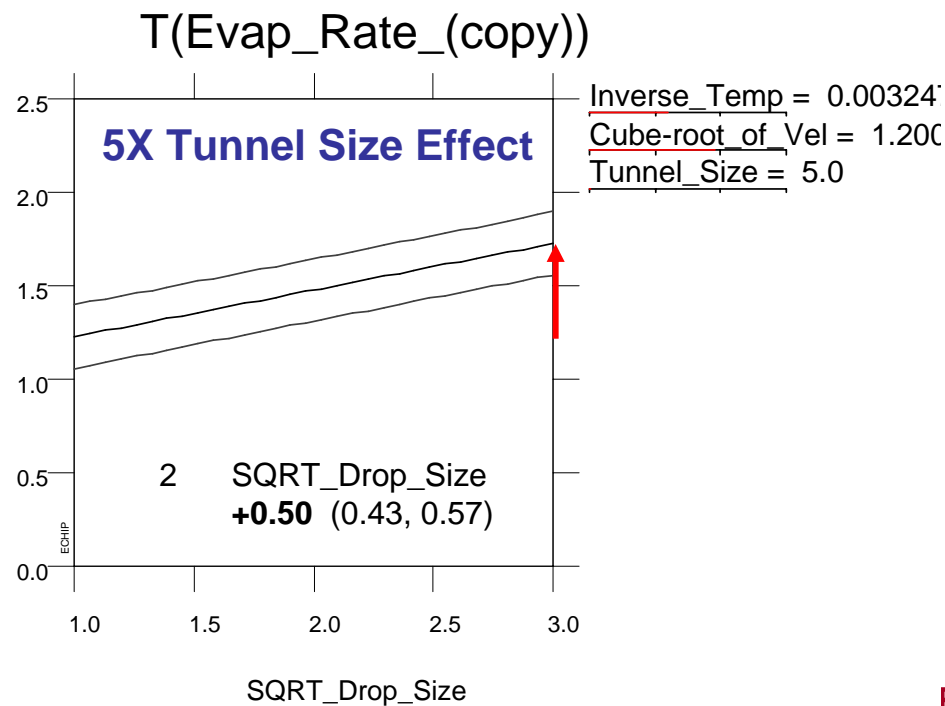
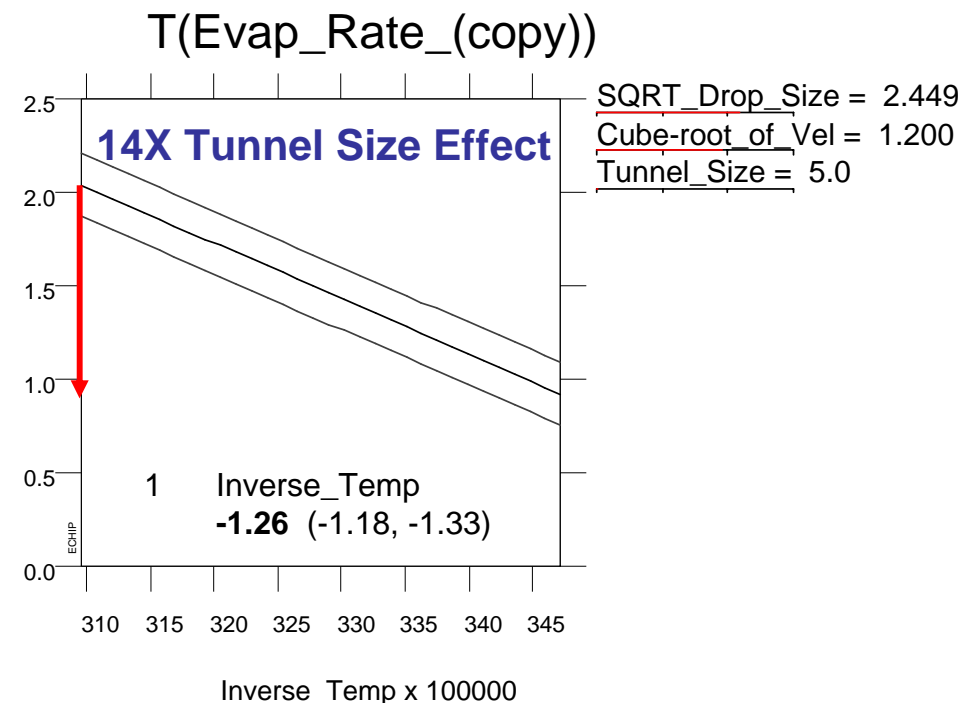
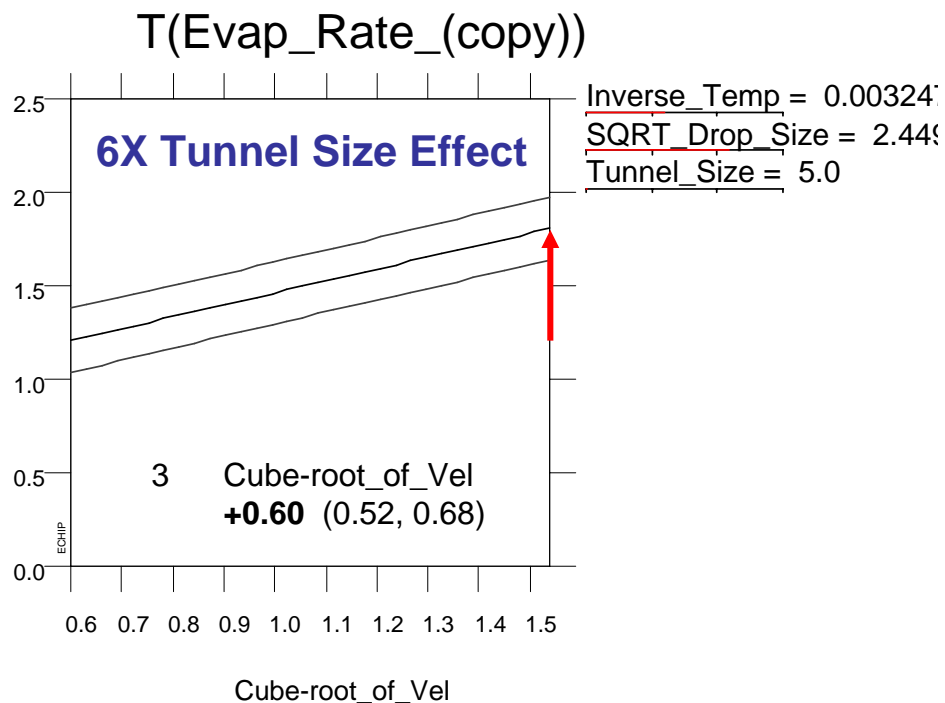
Pareto Effects for
 $\text{Log}_{10}(\text{Evap_Rate})$
5-cm tunnel



Pareto Effects for $\log_{10}(\text{Evap_Rate})$ including tunnel size (5-cm vs. 10-cm)



UNCLASSIFIED/UNLIMITED





Summary

- Rescaling the variables using knowledge of the physics reduces the complexity of the model required to adequately fit the data
 - Before rescaling, a 10-term quadratic model was needed
 - After rescaling, a 4-term linear model is all that is needed
- Extrapolated predictions for checkpoints within the 5-cm tunnel data validate “nearby” extrapolation with the physics-based linear model
- For the physics-based linear model “farther out” extrapolations are more plausible than those of the empirical model.
 - Note that these conditions are beyond the practical range of the wind tunnels and that these predictions have not been validated.



Summary

- Although the same level of reduction of the number of required trials seen for HD on glass may not hold true for other agents and/or substrates, results point to importance of running trials in a sequence of blocks that support increasingly complex models.
- Combining the data for the 5-cm and 10-cm tunnels shows that the “tunnel effect” - although statistically significant - is dwarfed by the effects of the Temperature, Wind Velocity and Drop Size which are 5X to 14X as large. For HD on glass, the behavior of the two tunnels appears quite similar.